LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM029010.D
Acq On : 05 Mar 2021 23:46
Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM029010.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.245	379	384	395	rVB	143912	208355	3.00%	0.206%
2	6.869	654	660	662	rBV	85523	136558	1.96%	0.135%
3	6.892	662	664	673	rVB	73553	101755	1.46%	0.101%
4	7.975	842	848	861	rVB	334250	508610	7.32%	0.504%
5	8.851	989	997	1005	rBV	167186	266103	3.83%	0.264%
6	9.128	1036	1044	1052	rBV3	64227	133088	1.91%	0.132%
7	9.322	1072	1077	1085	rBV	68976	123940	1.78%	0.123%
8	9.398	1085	1090	1105	rVB	142344	235304	3.38%	0.233%
9	9.886	1163	1173	1180	rVB	235347	407997	5.87%	0.404%
10	10.010	1187	1194	1208	rBV	409057	662982	9.54%	0.657%
11	10.469	1266	1272	1278	rBV	80315	149822	2.15%	0.148%
12	10.627	1295	1299	1315	rVB3	60971	157592	2.27%	0.156%
13	10.845	1329	1336	1344	rBV	60563	127898	1.84%	0.127%
14	10.922	1344	1349	1357	rVB	105051	179902	2.59%	0.178%
15	11.386	1413	1428	1437	rVB2	101602	373406	5.37%	0.370%
16	11.510	1442	1449	1461	rVB	140664	230387	3.31%	0.228%
17	11.857	1503	1508	1519	rVB	84450	144781	2.08%	0.143%
18	12.345	1586	1591	1605	rVB	78807	131202	1.89%	0.130%
19	12.563	1622	1628	1635	rVB	114835	167813	2.41%	0.166%
20	12.639	1635	1641	1645	rBV	181821	299725	4.31%	0.297%
21	12.704	1649	1652	1657	rVB	78031	107453	1.55%	0.106%
22	12.957	1689	1695	1706	rVB	398544	575360	8.28%	0.570%
23	13.321	1748	1757	1764	rBV	1157761	1727791	24.85%	1.712%
24	13.733	1822	1827	1832	rBV	91004	130548	1.88%	0.129%
25	13.874	1844	1851	1854	rBV	92562	142868	2.05%	0.142%
26	14.345	1925	1931	1936	rVV	109774	163922	2.36%	0.162%
27	14.404	1936	1941	1948	rVB	579740	762796	10.97%	0.756%
28	15.239	2077	2083	2088	rBV	89200	126328	1.82%	0.125%
29	15.362	2099	2104	2109	rBV	166949	224017	3.22%	0.222%
30	15.415	2109	2113	2120	rVB	247077	320297	4.61%	0.317%
31	15.845	2180	2186	2190	rBV	372591	504365	7.25%	0.500%
32	16.015	2206	2215	2221	rBV	2466920	3715046	53.43%	3.682%
33	16.080	2222	2226	2239	rVB	113126	178824	2.57%	0.177%
34	16.262	2252	2257	2264	rVB	222216	276970	3.98%	0.274%
35	16.656	2317	2324	2328	rBV4	78556	170043	2.45%	0.169%
36	16.815	2345	2351	2356	rBV	1614786	2096155	30.15%	2.077%

LSC Area Percent Report

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Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	17.045	2385	2390	2394	rBV2	108017	149326	2.15%	0.148%
38	17.092	2394	2398	2403	rVV	112492	143794	2.07%	0.143%
39	17.280	2426	2430	2434	rBV	91129	109899	1.58%	0.109%
40	17.433	2452	2456	2461	rVB	111795	146154	2.10%	0.145%
41	17.568	2473	2479	2490	rVB3	689390	1277088	18.37%	1.266%
42	17.939	2538	2542	2548	rVV	109466	139614	2.01%	0.138%
43	18.009	2549	2554	2559	rVV	129995	167812	2.41%	0.166%
44	18.092	2559	2568	2571	rVV	3537327	5551663	79.85%	5.502%
45	18.115	2571	2572	2584	rVB	197855	192567	2.77%	0.191%
46	18.268	2593	2598	2603	rBV	362443	446416	6.42%	0.442%
47	18.509	2634	2639	2643	rVV	82651	109288	1.57%	0.108%
48	18.574	2644	2650	2659	rVB2	127402	203423	2.93%	0.202%
49	18.750	2672	2680	2690	rBV	2767019	3877876	55.77%	3.843%
50	18.903	2702	2706	2714	rVB	197436	245314	3.53%	0.243%
51	19.098	2734	2739	2747	rBV	113926	153844	2.21%	0.152%
52	19.186	2749	2754	2757	rVV2	70019	101677	1.46%	0.101%
53	19.227	2757	2761	2767	rVB	137995	171108	2.46%	0.170%
54	19.350	2776	2782	2791	rVB	1669166	2115471	30.43%	2.097%
55	19.580	2816	2821	2824	rBV	107611	158647	2.28%	0.157%
56	19.615	2824	2827	2834	rVB	155542	189098	2.72%	0.187%
57	19.721	2839	2845	2847	rBV	684587	860564	12.38%	0.853%
58	19.768	2847	2853	2867	rVB	4419054	6769784	97.37%	6.709%
59	19.886	2868	2873	2878	rBV	488690	555777	7.99%	0.551%
60	20.056	2897	2902	2908	rVV	143103	217370	3.13%	0.215%
61	20.115	2908	2912	2920	rVB2	144061	253296	3.64%	0.251%
62	20.286	2933	2941	2945	rBV	3711425	5060706	72.79%	5.015%
63	20.392	2955	2959	2965	rVB	272637	320838	4.61%	0.318%
64	20.544	2981	2985	2989	rBV	99128	116976	1.68%	0.116%
65	20.609	2992	2996	3000	rBV2	52869	99450	1.43%	0.099%
66	20.650	3000	3003	3007	rVB	123666	133595	1.92%	0.132%
67	20.762	3016	3022	3027	rBV	2285474	2772534	39.88%	2.748%
68	20.956	3052	3055	3064	rVB2	175222	330347	4.75%	0.327%
69	21.103	3071	3080	3086	rBV	4872551	6952949	100.00%	6.891%
70	21.191	3091	3095	3100	rVV	517240	586657	8.44%	0.581%
71	21.268	3103	3108	3113	rVV	170867	288490	4.15%	0.286%
72	21.315	3113	3116	3120	rVV	128744	151487	2.18%	0.150%
73	21.368	3121	3125	3129	rVB	169985	211498	3.04%	0.210%
74	21.533	3144	3153	3162	rBV	3882673	5480902	78.83%	5.432%
75	21.609	3162	3166	3174	rVB	295324	365070	5.25%	0.362%
76	21.844	3199	3206	3211	rVB	98542	166263	2.39%	0.165%

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Misc :
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Instrument : BNA_M
ClientSampleId : 435-416

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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Stop Thrs : 0 Peak Location: TOP

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Peak separation: 5

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77	21.950	3218	3224	3233	rBV	1874916	2724293	39.18%	2.700%
78	22.127	3251	3254	3262	rVB	117314	189247	2.72%	0.188%
79	22.291	3273	3282	3290	rBV	3627689	6060009	87.16%	6.006%
80	22.380	3293	3297	3307	rVB	374416	512454	7.37%	0.508%
81	22.503	3314	3318	3323	rVB	97047	153701	2.21%	0.152%
82	22.562	3323	3328	3334	rVB	136806	216172	3.11%	0.214%
83	22.774	3352	3364	3375	rBV	2645051	4725143	67.96%	4.683%
84	22.868	3376	3380	3391	rVB	171422	282747	4.07%	0.280%
85	23.162	3424	3430	3439	rVB2	70651	147213	2.12%	0.146%
86	23.309	3445	3455	3464	rBV	1023913	2000096	28.77%	1.982%
87	23.433	3471	3476	3481	rVB2	99609	166490	2.39%	0.165%
88	23.527	3488	3492	3498	rVB	59417	99716	1.43%	0.099%
89	23.756	3519	3531	3545	rBV	2198191	5080012	73.06%	5.034%
90	23.874	3545	3551	3566	rVV	222513	465893	6.70%	0.462%
91	24.032	3569	3578	3585	rVV3	69438	231273	3.33%	0.229%
92	24.115	3587	3592	3604	rVB	81492	180188	2.59%	0.179%
93	24.432	3634	3646	3657	rVV	1584656	3824572	55.01%	3.790%
94	24.556	3661	3667	3675	rVB	84069	188362	2.71%	0.187%
95	25.197	3763	3776	3791	rVB	531671	1505570	21.65%	1.492%
96	25.862	3873	3889	3905	rBV	1062401	3407088	49.00%	3.377%
97	26.032	3911	3918	3930	rVB	94346	264549	3.80%	0.262%
98	26.879	4047	4062	4081	rVB	709358	2626839	37.78%	2.603%
99	28.068	4255	4264	4280	rVB2	196577	760139	10.93%	0.753%
100	29.091	4420	4438	4461	rVB2	364351	1777747	25.57%	1.762%

Sum of corrected areas: 100904148

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Instrument :
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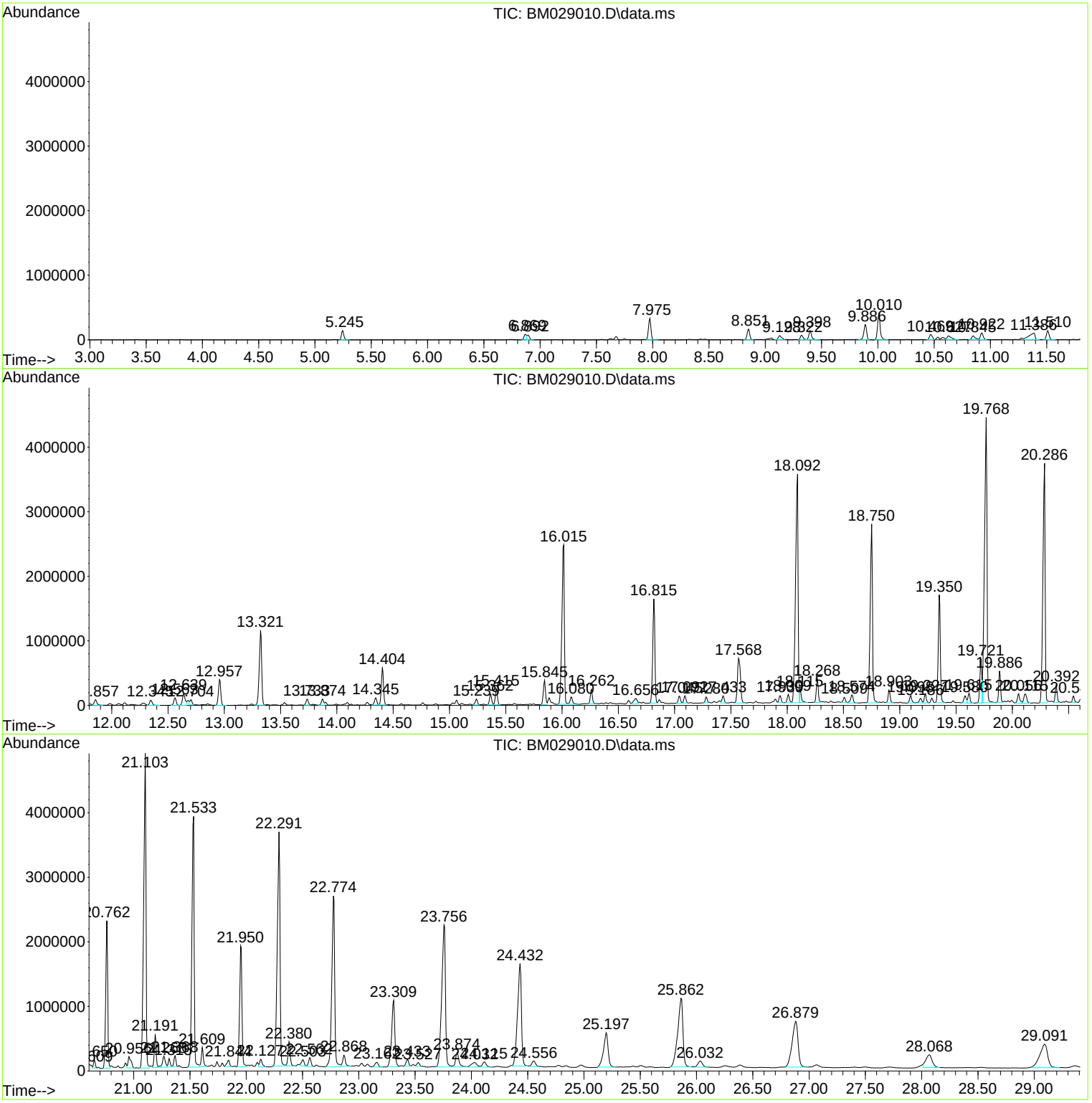
ClientSampleId :
435-416

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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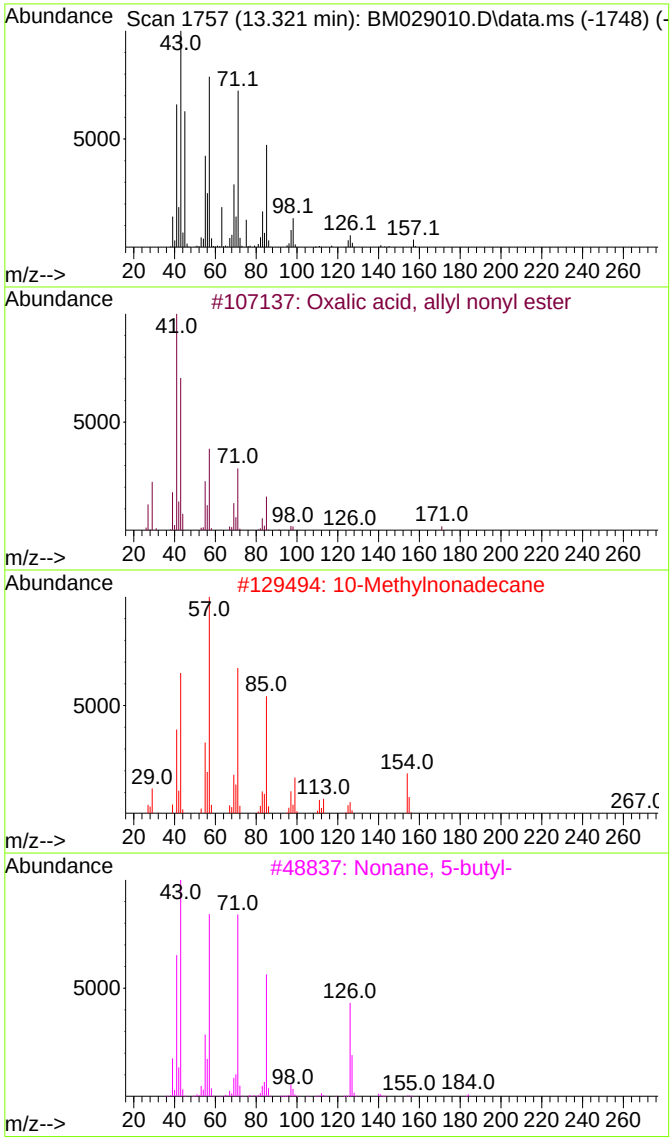
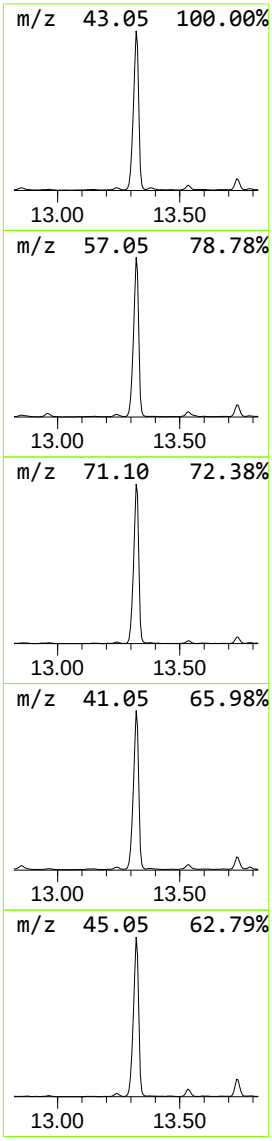
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Oxalic acid, allyl nonyl ester Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.321	210.81 ng	1727790	Acenaphthene-d10	14.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	62
2	10-Methylnonadecane	282	C20H42	056862-62-5	50
3	Nonane, 5-butyl-	184	C13H28	017312-63-9	50
4	Decane, 3-methyl-	156	C11H24	013151-34-3	47
5	Sulfurous acid, butyl nonyl ester	264	C13H28O3S	1000309-17-6	47





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Instrument : BNA_M
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

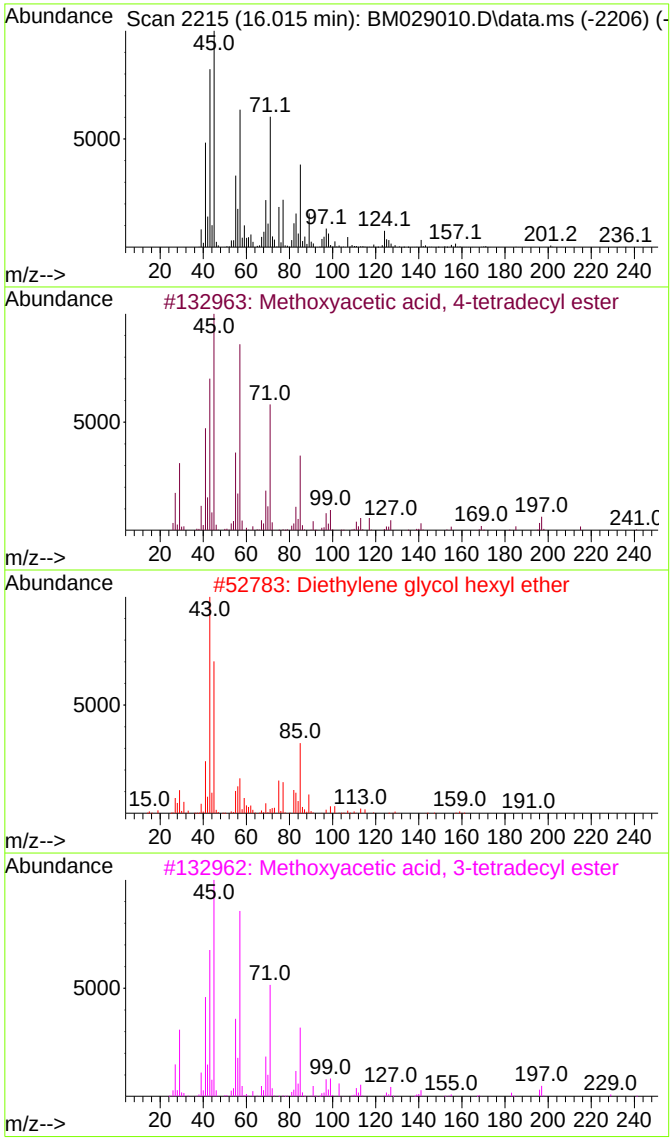
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

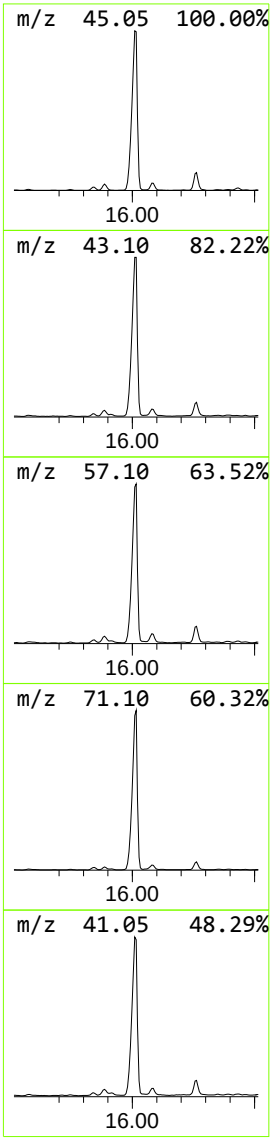
****

Peak Number 2 Methoxyacetic acid, 4-tetra... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.015	516.72 ng	3715050	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 4-tetradecyl...	286	C17H34O3	1000282-05-0	58
2	Diethylene glycol hexyl ether	190	C10H22O3	000112-59-4	58
3	Methoxyacetic acid, 3-tetradecyl...	286	C17H34O3	1000282-04-9	53
4	Methoxyacetic acid, 2-pentyl ester	160	C8H16O3	1000282-69-2	47
5	Methoxyacetic acid, 3-tridecyl e...	272	C16H32O3	1000282-04-6	43





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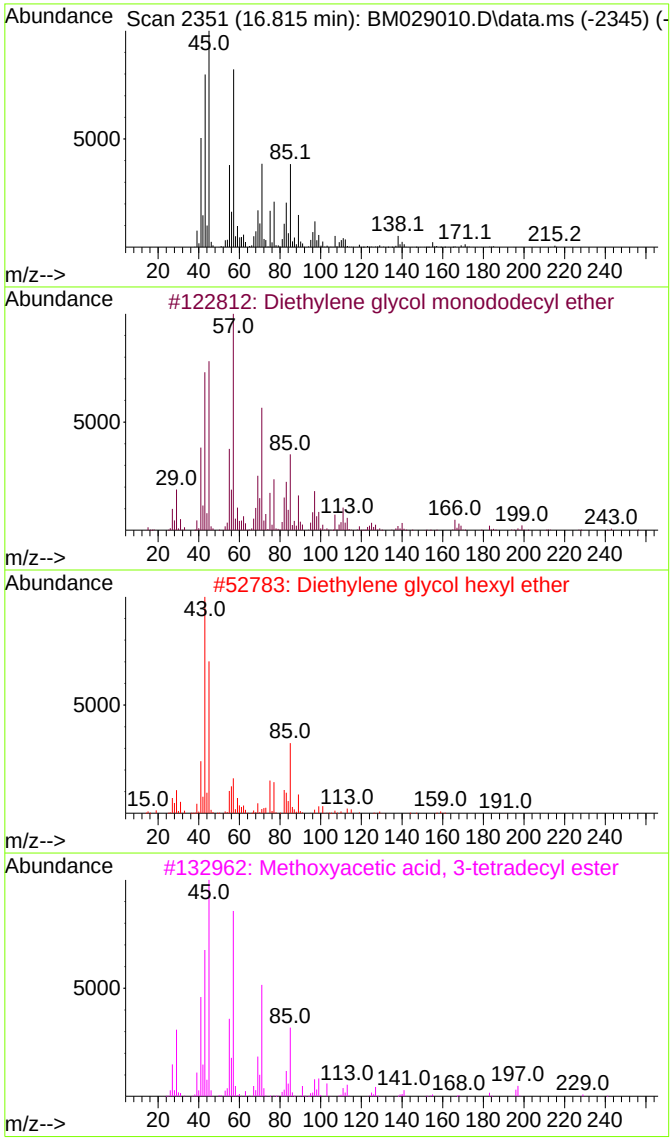
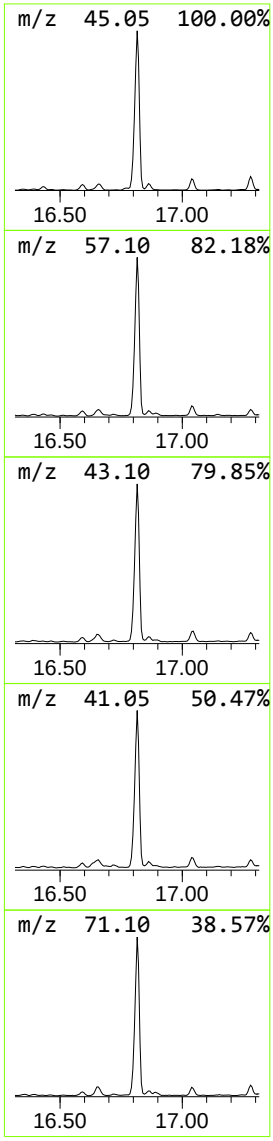
****
Peak Number 3 Diethylene glycol monododec... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.815	291.55 ng	2096160	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Diethylene glycol monododecyl ether	274	C16H34O3	003055-93-4	64
2	Diethylene glycol hexyl ether	190	C10H22O3	000112-59-4	58
3	Methoxyacetic acid, 3-tetradecyl...	286	C17H34O3	1000282-04-9	52
4	Methoxyacetic acid, 3-tridecyl e...	272	C16H32O3	1000282-04-6	50
5	Methoxyacetic acid, 2-tridecyl e...	272	C16H32O3	1000282-04-5	46





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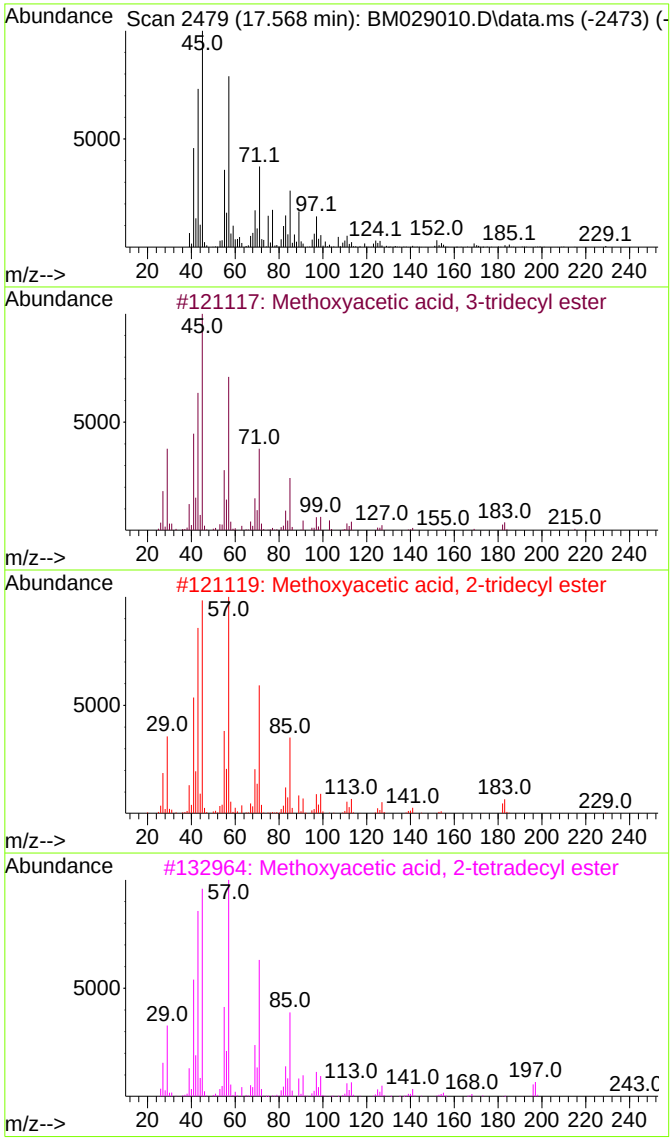
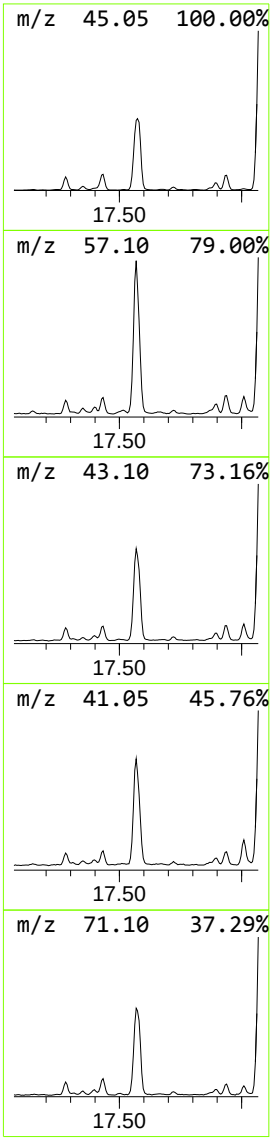
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Methoxyacetic acid, 3-tride... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.568	177.63 ng	1277090	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Methoxyacetic acid, 3-tridecyl e...	272	C16H32O3	1000282-04-6	72
2	Methoxyacetic acid, 2-tridecyl e...	272	C16H32O3	1000282-04-5	52
3	Methoxyacetic acid, 2-tetradecyl...	286	C17H34O3	1000282-04-8	52
4	2-Tetradecanol	214	C14H30O	004706-81-4	50
5	2-Hexanol, 3,4-dimethyl-	130	C8H18O	019550-05-1	50





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Instrument :
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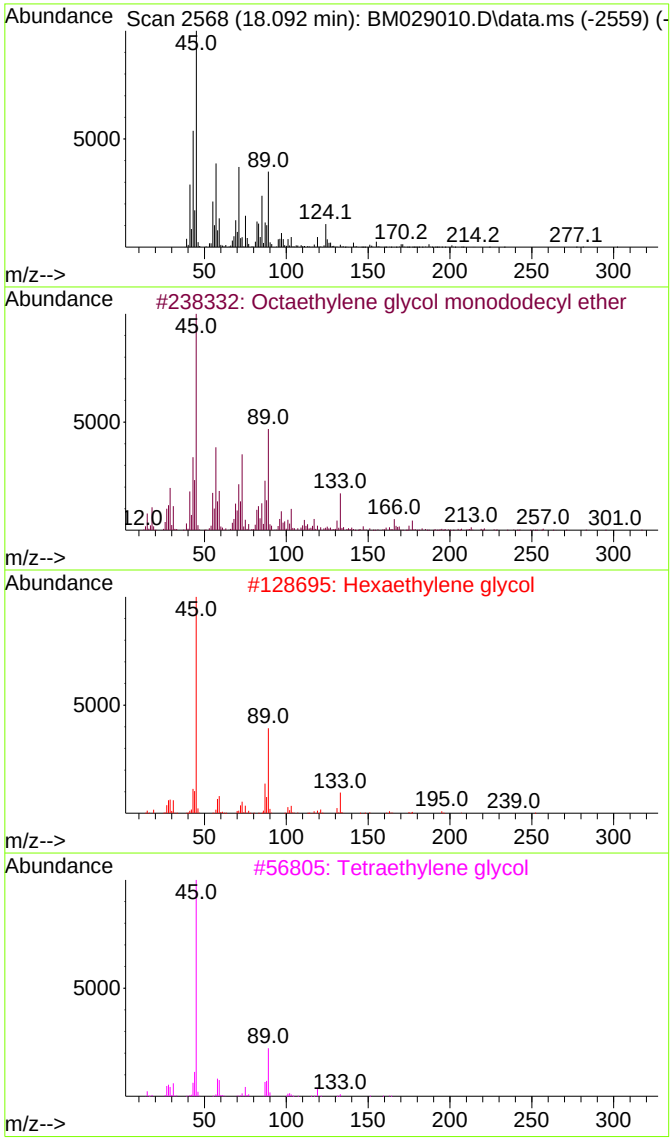
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

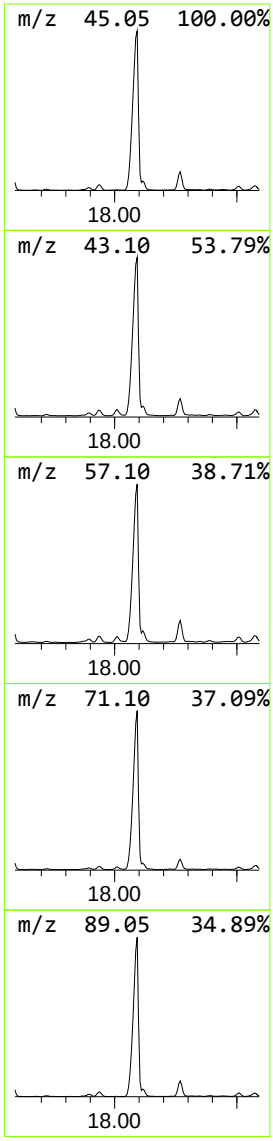
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Octaethylene glycol monodod... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.092	772.17 ng	5551660	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octaethylene glycol monododecyl ...	538	C28H58O9	003055-98-9	59
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	58
3	Tetraethylene glycol	194	C8H18O5	000112-60-7	53
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	53
5	Pentaethylene glycol	238	C10H22O6	004792-15-8	53





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Acq On : 05 Mar 2021 23:46
Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

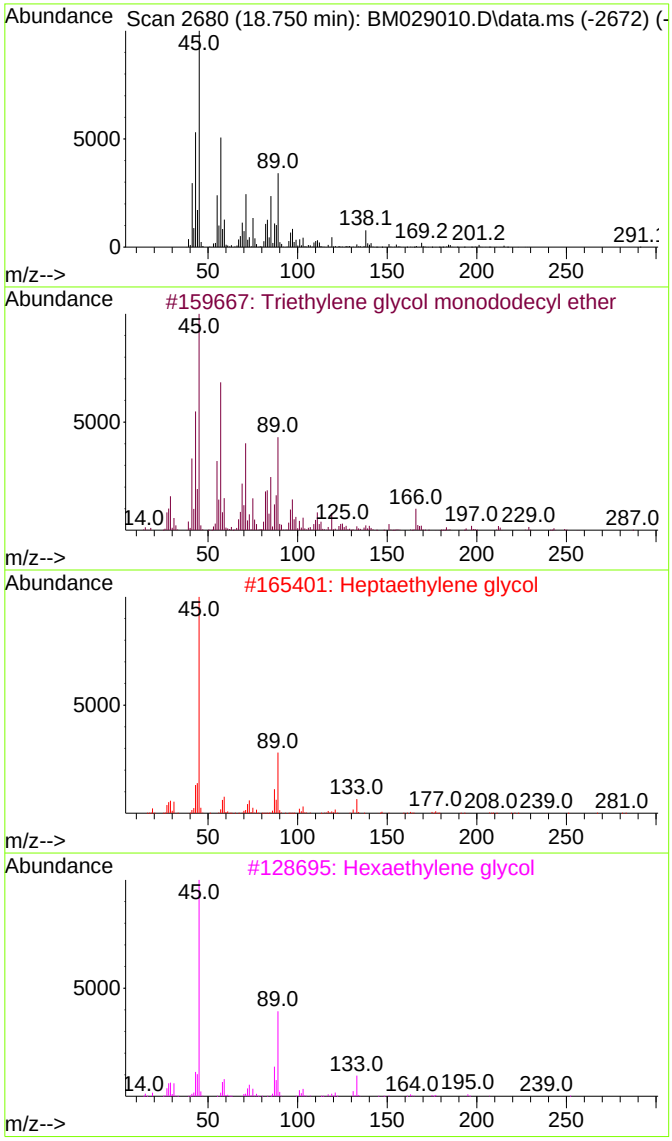
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

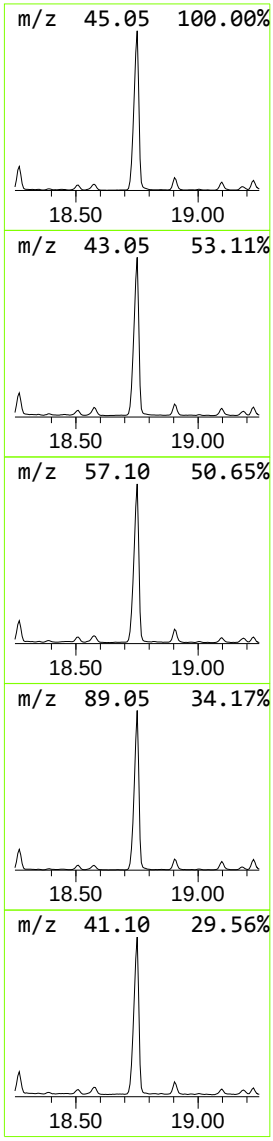
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Triethylene glycol monodode... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.750	539.37 ng	3877880	Phenanthrene-d10	17.092

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethylene glycol monododecyl e...	318	C18H38O4	003055-94-5	87
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	58
3	Hexaethylene glycol	282	C12H26O7	002615-15-8	58
4	Pentaethylene glycol	238	C10H22O6	004792-15-8	53
5	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	53





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Acq On : 05 Mar 2021 23:46
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Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

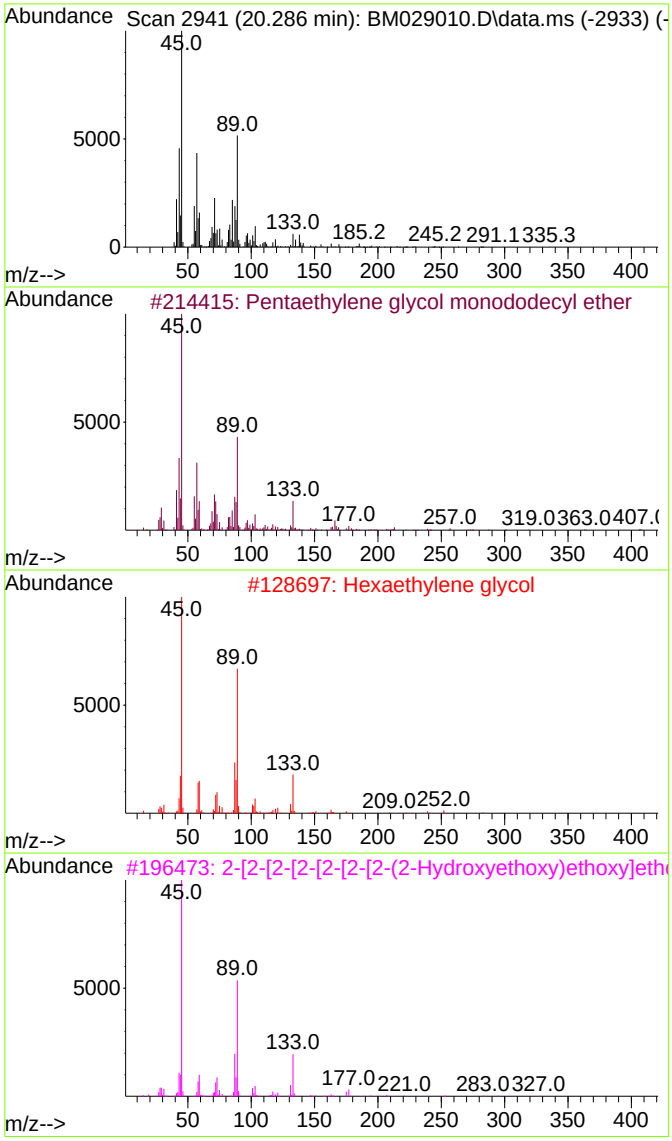
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

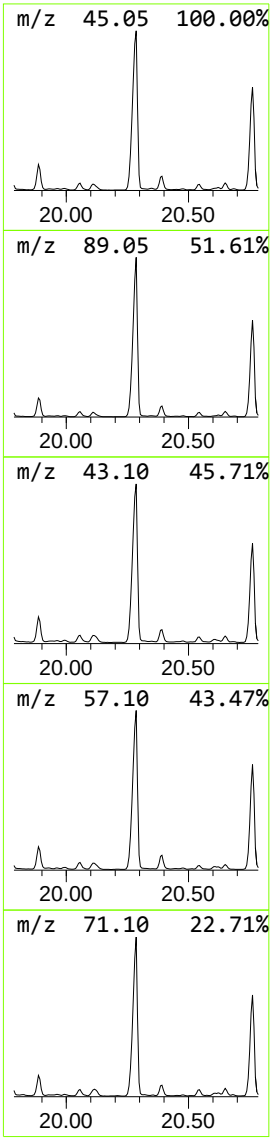
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 7 Pentaethylene glycol monodo... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.286	350.84 ng	5060710	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	80
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	68
3	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	64
4	Tetraethylene glycol	194	C8H18O5	000112-60-7	58
5	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	58





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Operator : CG/JU
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
435-416

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

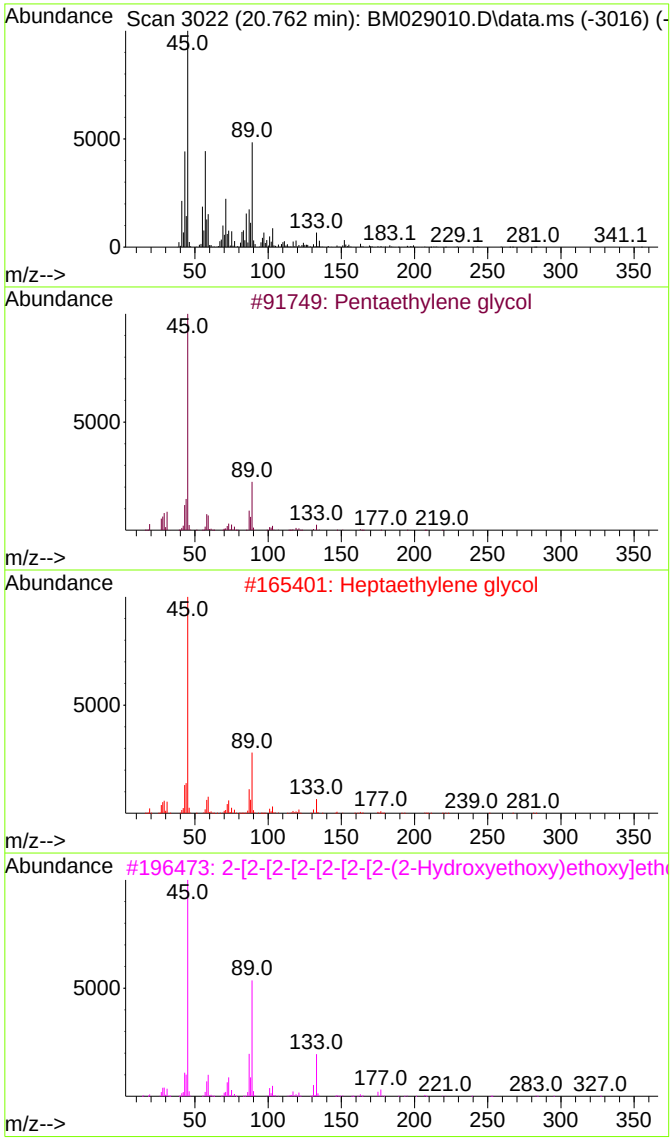
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

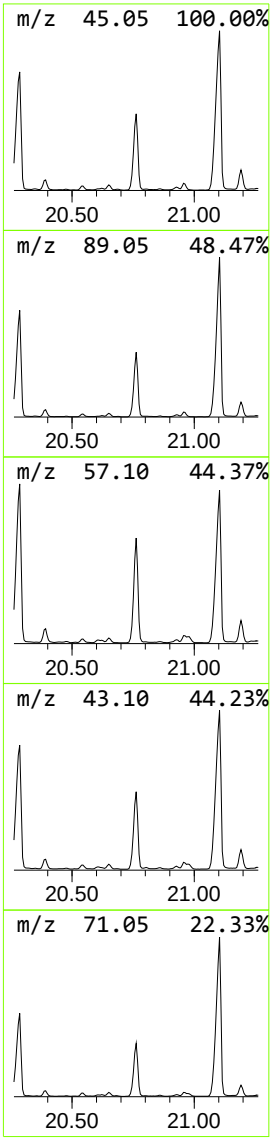
****

Peak Number 8 Pentaethylene glycol Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.762	192.21 ng	2772530	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol	238	C10H22O6	004792-15-8	80
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	80
3	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	74
4	Hexaethylene glycol	282	C12H26O7	002615-15-8	72
5	Tetraethylene glycol	194	C8H18O5	000112-60-7	64





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Acq On : 05 Mar 2021 23:46
Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
435-416

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

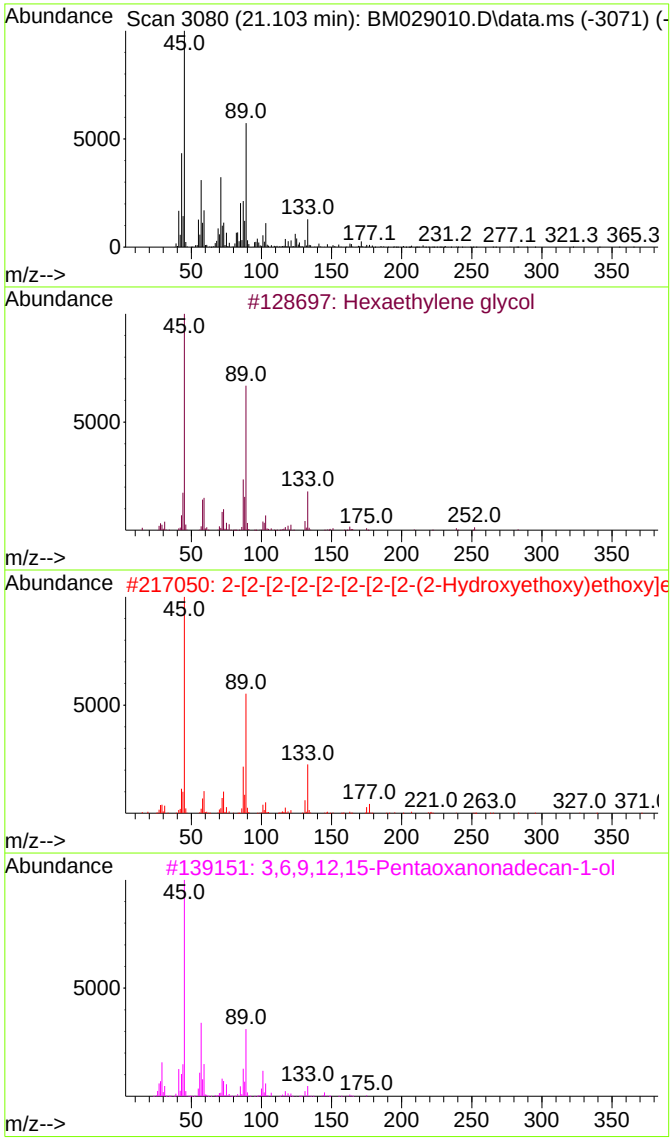
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

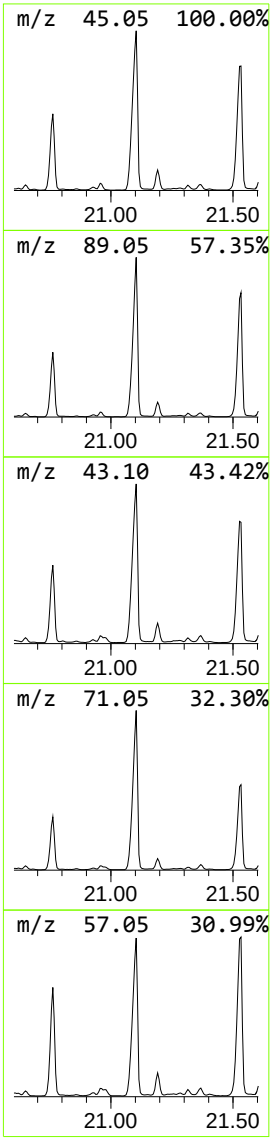
****

Peak Number 9 Hexaethylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.103	482.02 ng	6952950	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol	282	C12H26O7	002615-15-8	74
2	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	74
3	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	72
4	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	72
5	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	72





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Acq On : 05 Mar 2021 23:46
Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

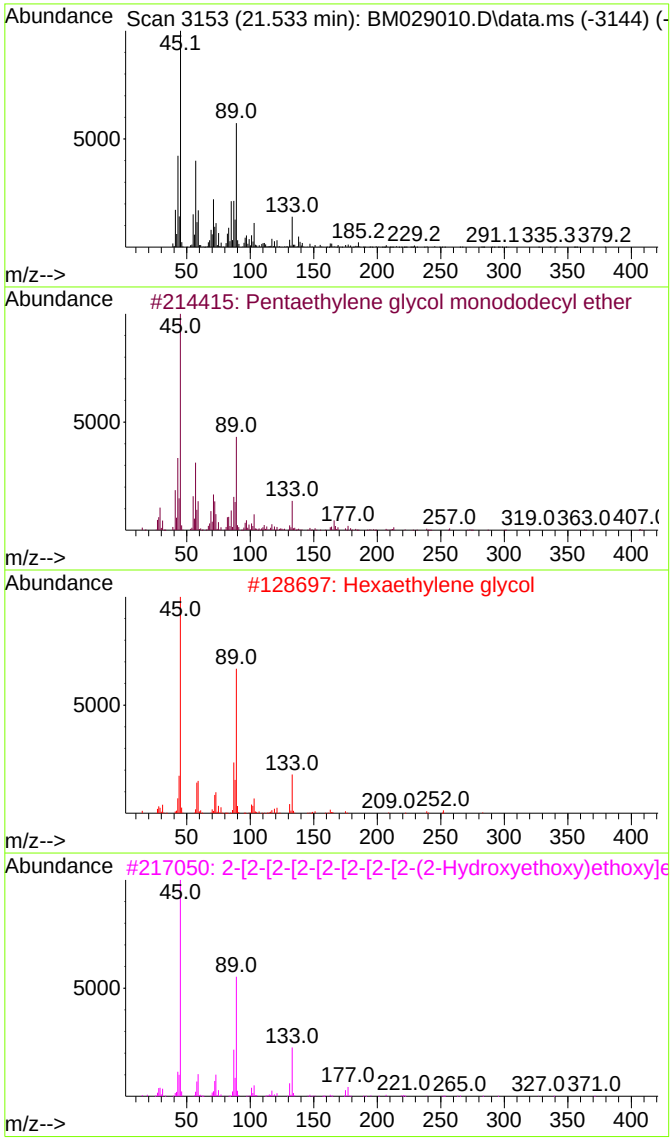
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

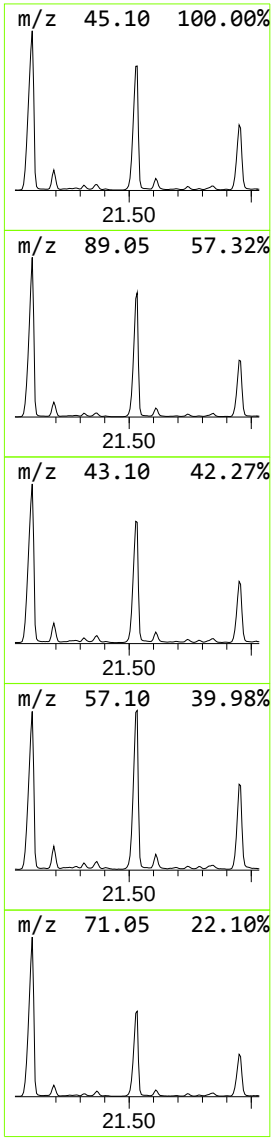
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 2-[2-[2-[2-[2-[2-[2-[2-(2-H... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.533	379.97 ng	5480900	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	87
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	81
3	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	74
4	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	74
5	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	74





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Acq On : 05 Mar 2021 23:46
Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

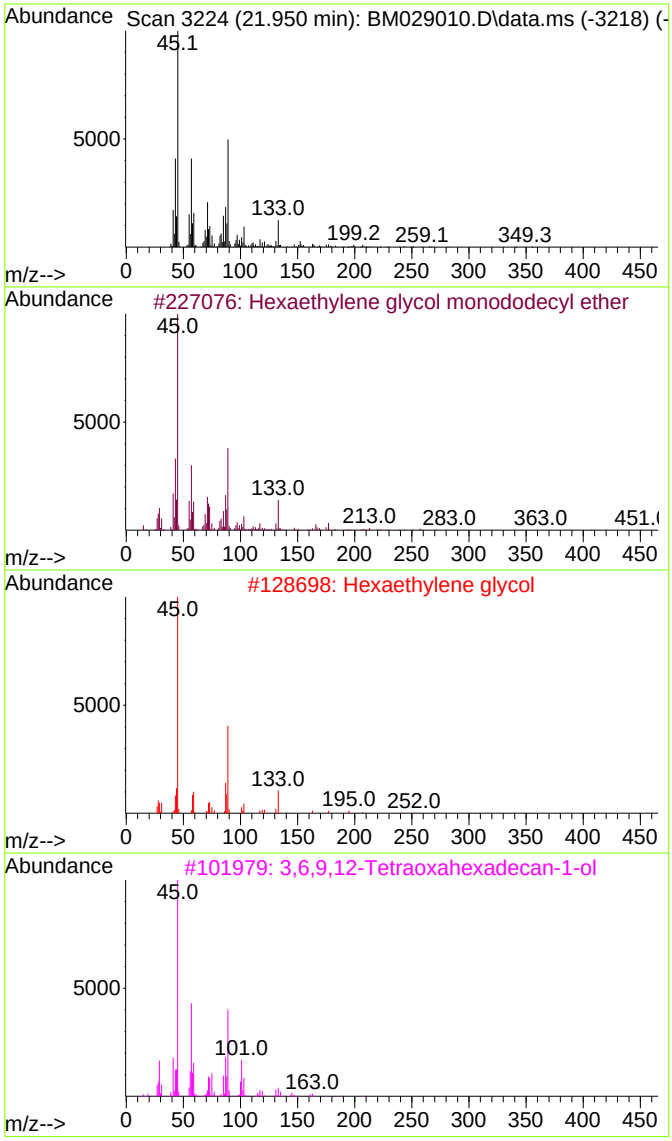
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

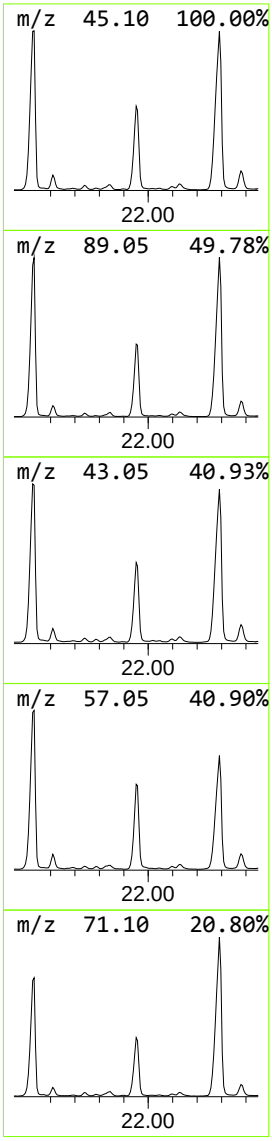
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 Hexaethylene glycol monodod... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.950	188.87 ng	2724290	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	90
2	Hexaethylene glycol	282	C12H26O7	002615-15-8	83
3	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	83
4	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	74
5	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	72





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Acq On : 05 Mar 2021 23:46
Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
435-416

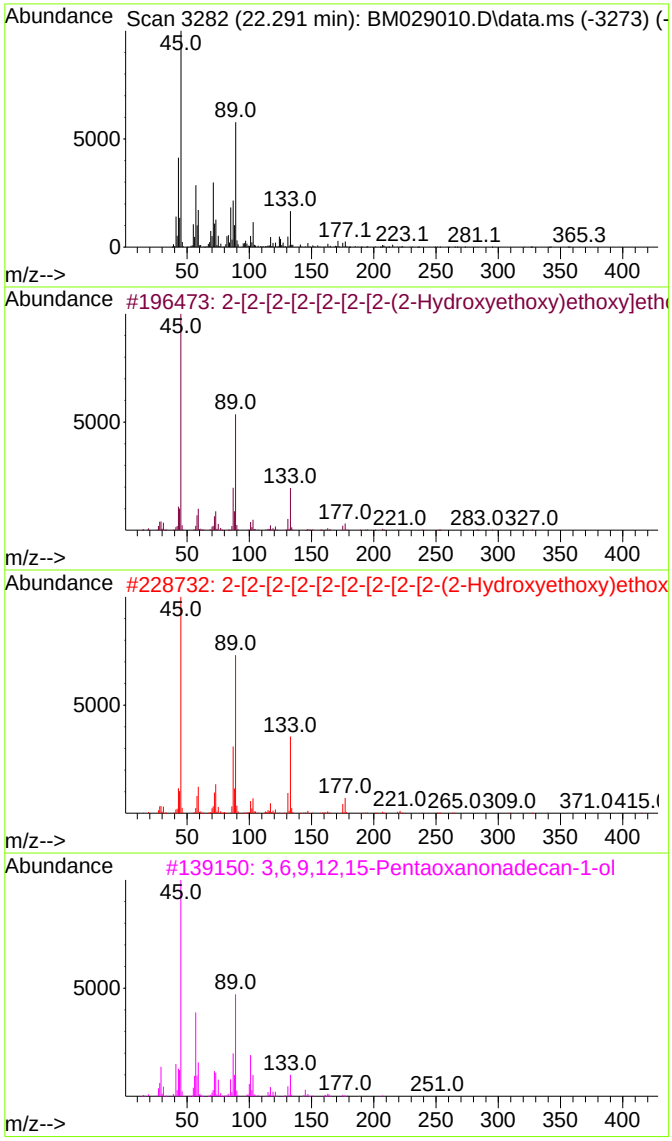
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

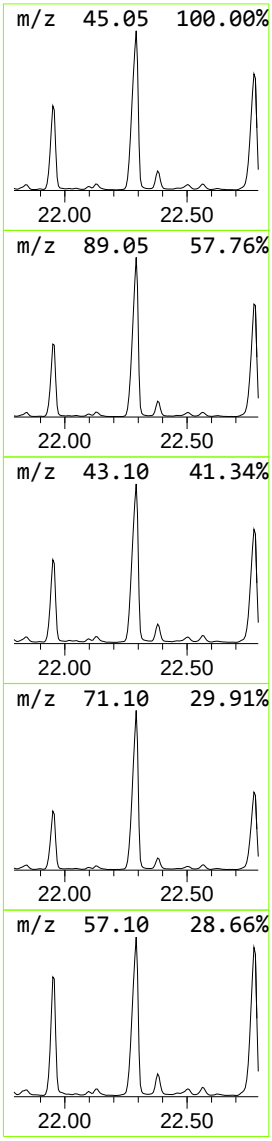
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 2-[2-[2-[2-[2-[2-[2-(2-Hydr... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.291	420.12 ng	6060010	Chrysene-d12	21.268

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	87
2	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	83
3	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	83
4	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	83
5	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	83





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Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

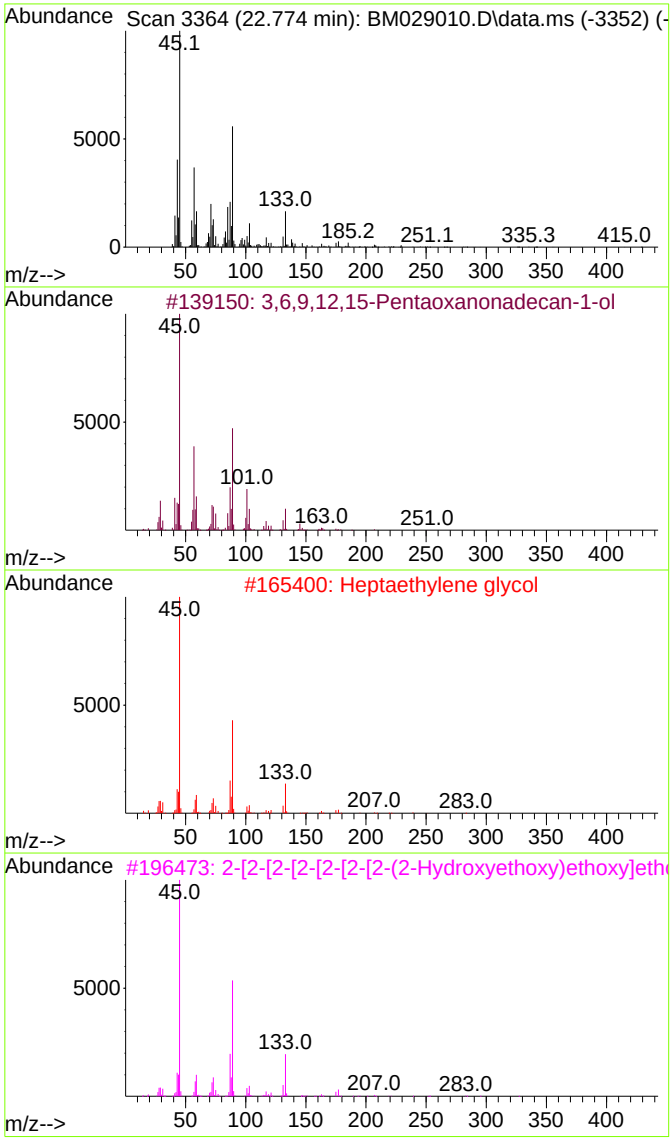
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

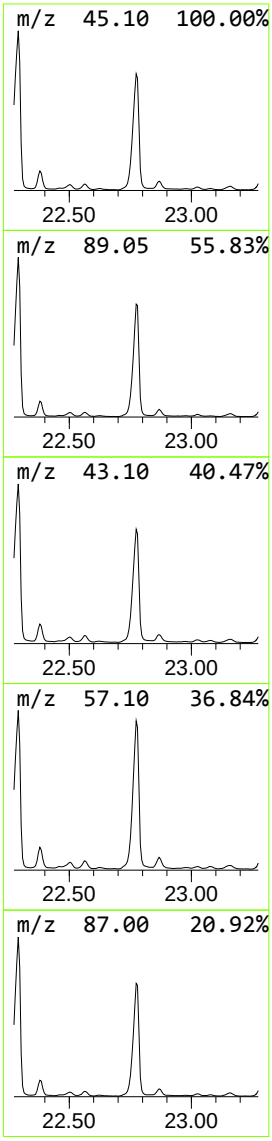
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 13 3,6,9,12,15-Pentaoxanonadec... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.774	567.62 ng	4725140	Perylene-d12	23.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	87
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	87
3	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	87
4	2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	83
5	2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	83





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Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
435-416

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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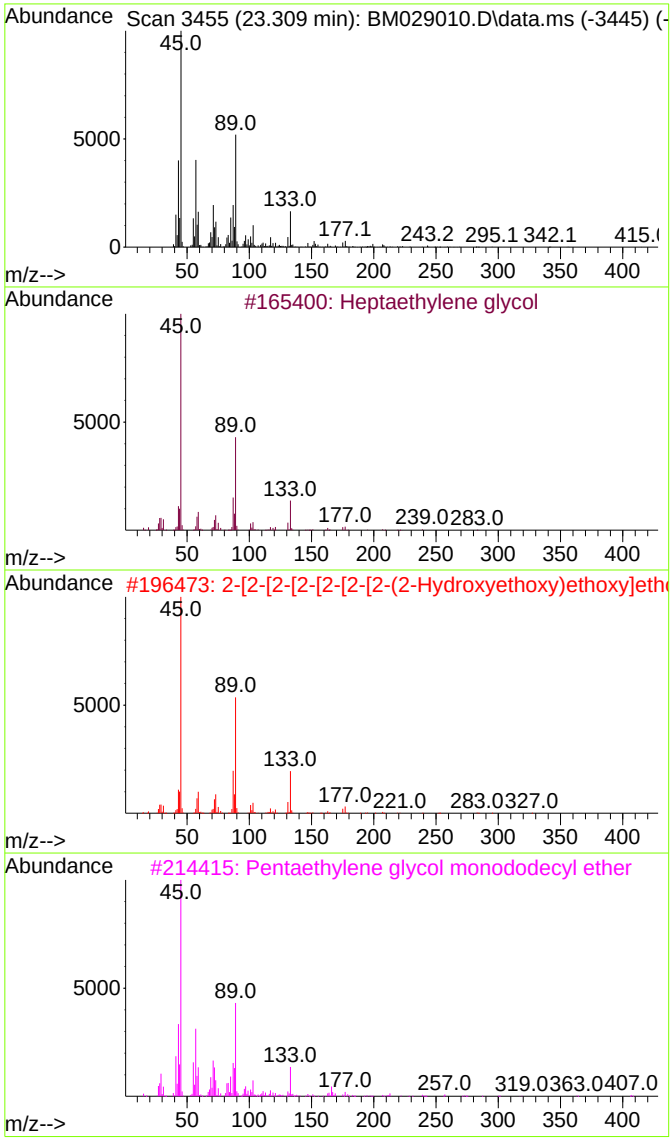
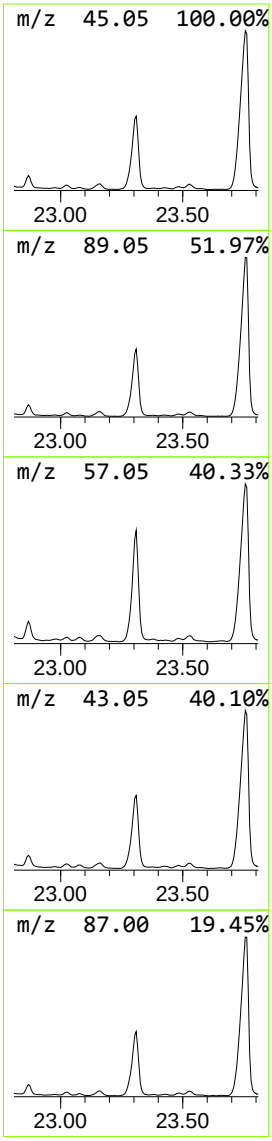
Peak Number 14 Heptaethylene glycol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.309	240.27 ng	2000100	Perylene-d12	23.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol	326	C14H30O8	005617-32-3	87
2	2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	87
3	Pentaethylene glycol monododecyl...	406	C22H46O6	003055-95-6	86
4	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	83
5	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	83





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Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

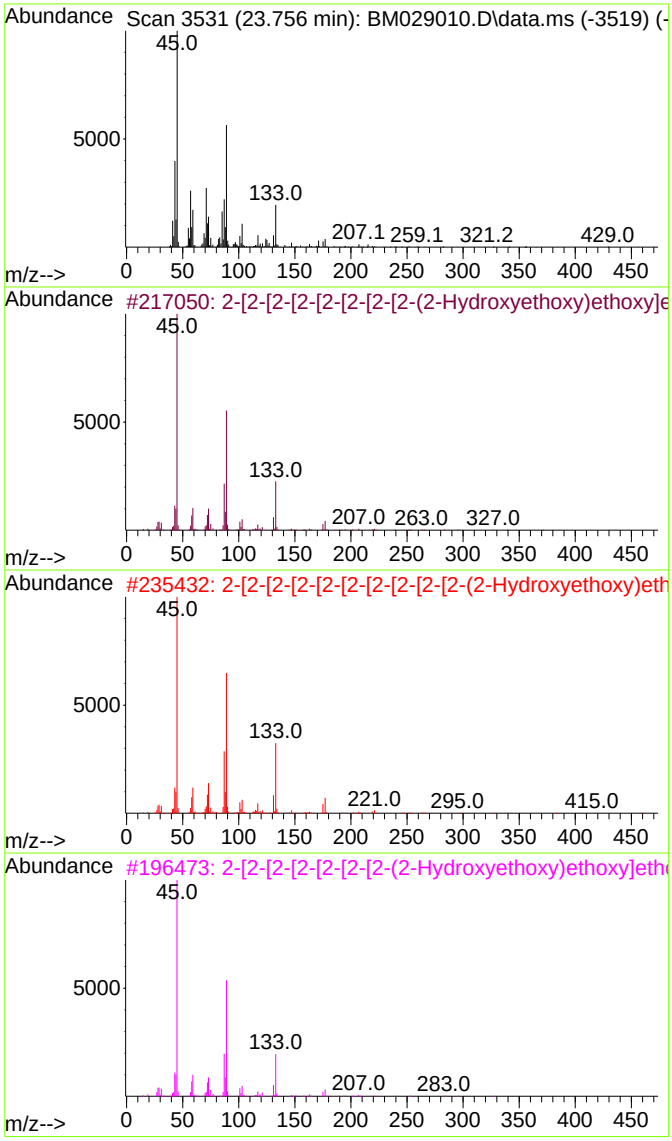
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

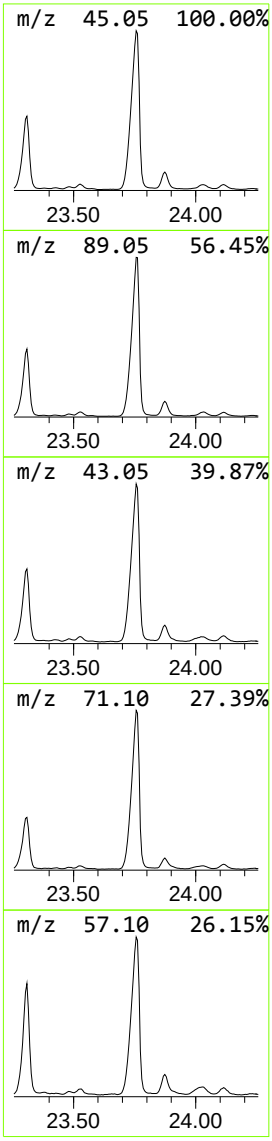
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 15 2-[2-[2-[2-[2-[2-[2-[2-[2-[... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.756	610.25 ng	5080010	Perylene-d12	23.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	87
2	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	87
3	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	87
4	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	87
5	2-[2-[2-[2-[2-[2-[2-[2-[2-(2-Hyd...	458	C20H42O11	1000352-12-6	83





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Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
435-416

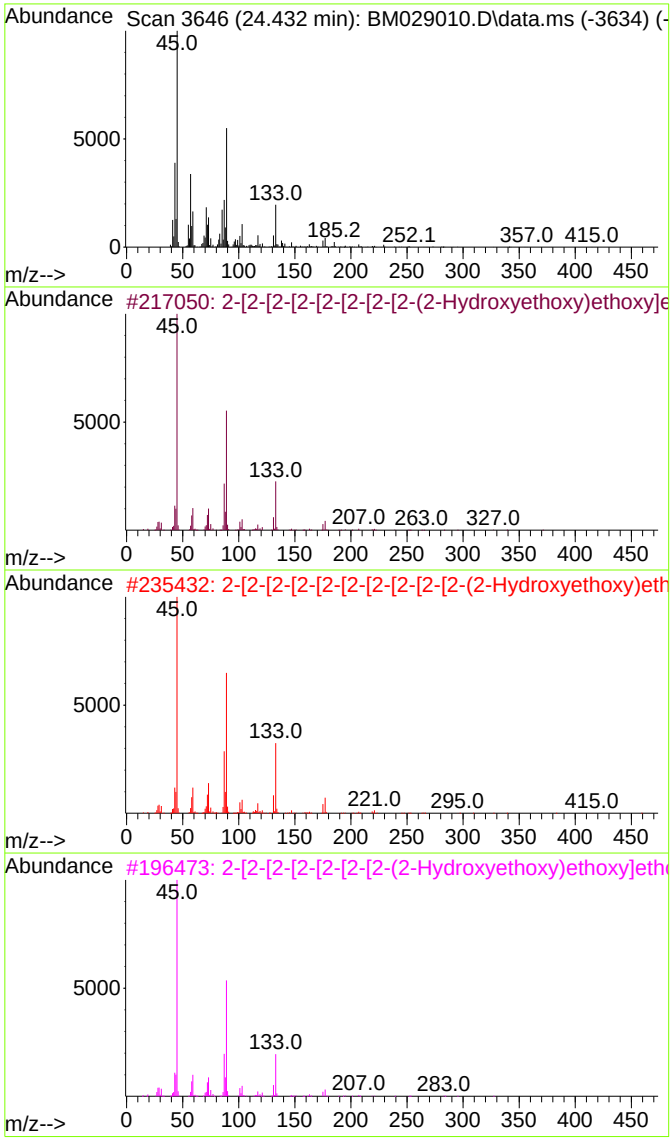
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

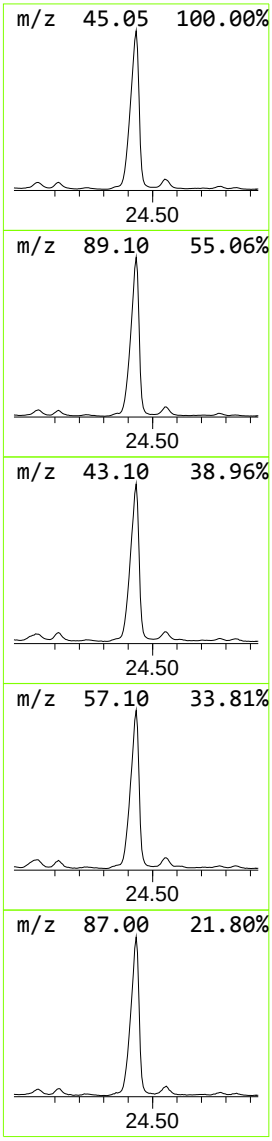
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 16 2-[2-[2-[2-[2-[2-[2-[2-[2-[... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.433	459.44 ng	3824570	Perylene-d12	23.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	90
2	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	90
3	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	90
4	Heptaethylene glycol	326	C14H30O8	005617-32-3	87
5	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM029010.D
Acq On : 05 Mar 2021 23:46
Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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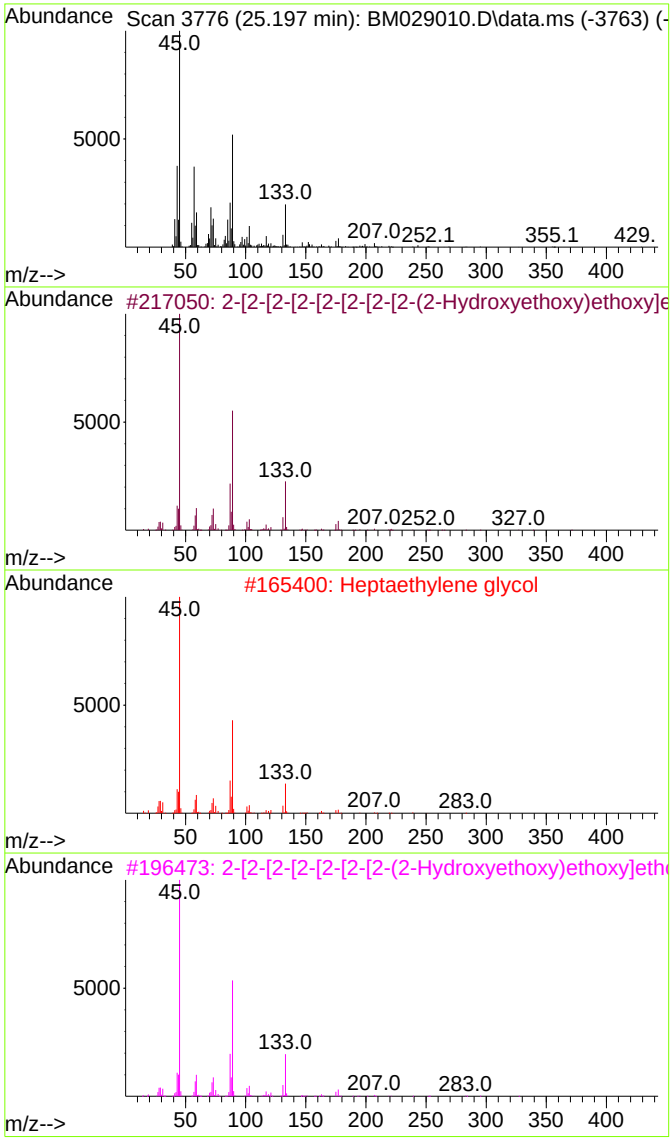
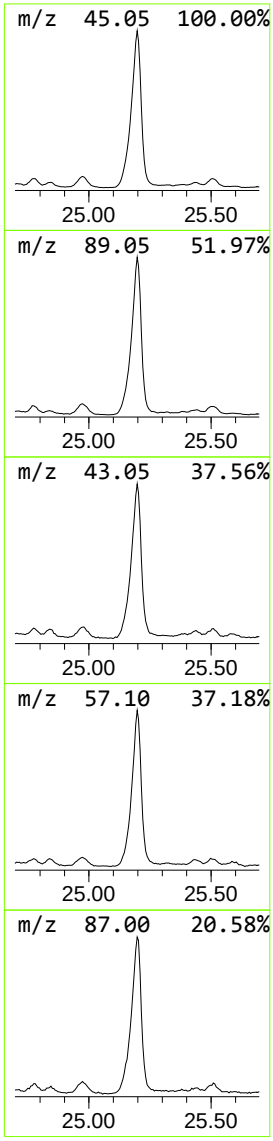
Peak Number 17 unknown25.197 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.197	180.86 ng	1505570	Perylene-d12	23.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	90
2	Heptaethylene glycol	326	C14H30O8	005617-32-3	90
3	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	90
4	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	90
5	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM029010.D
Acq On : 05 Mar 2021 23:46
Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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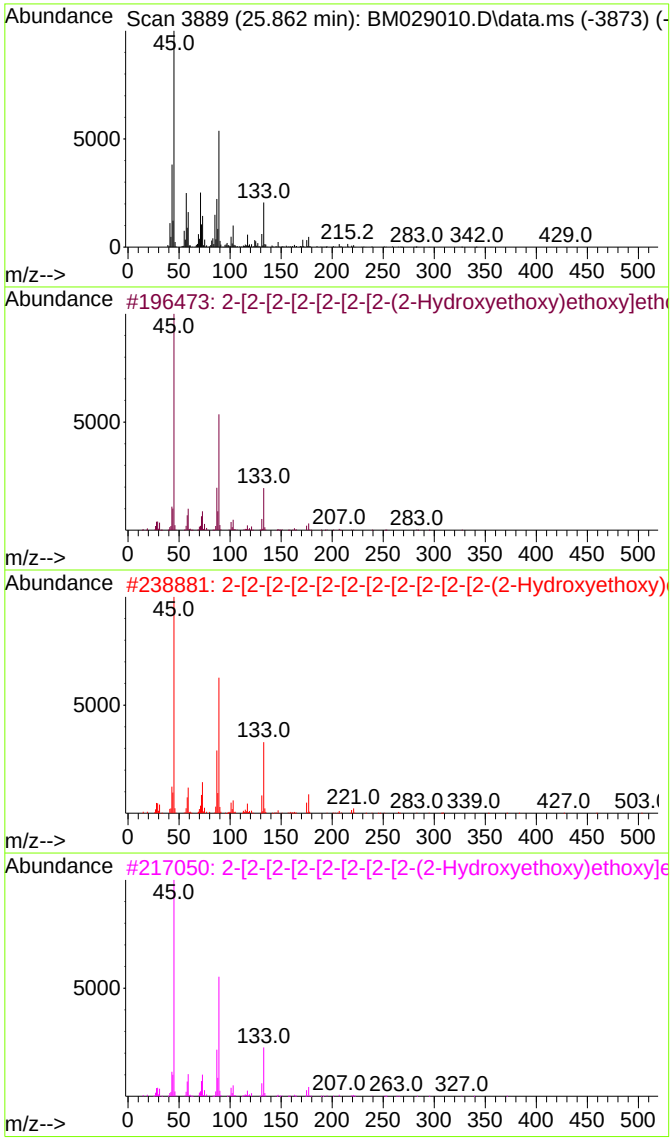
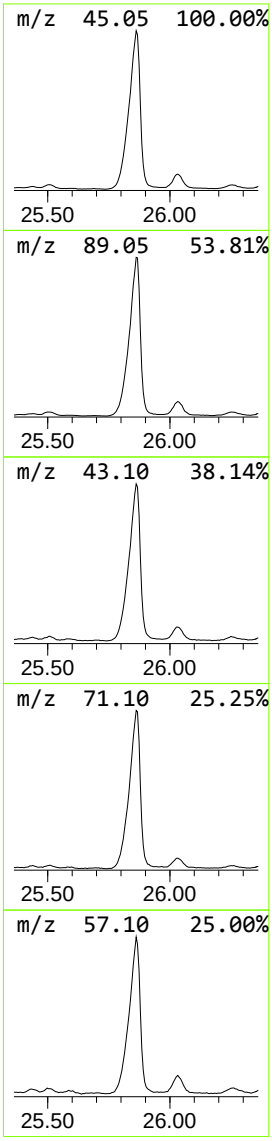
Peak Number 18 unknown25.862 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.862	409.28 ng	3407090	Perylene-d12	23.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	87
2	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	87
3	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	87
4	Hexaethylene glycol monododecyl ...	450	C24H50O7	003055-96-7	78
5	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM029010.D
Acq On : 05 Mar 2021 23:46
Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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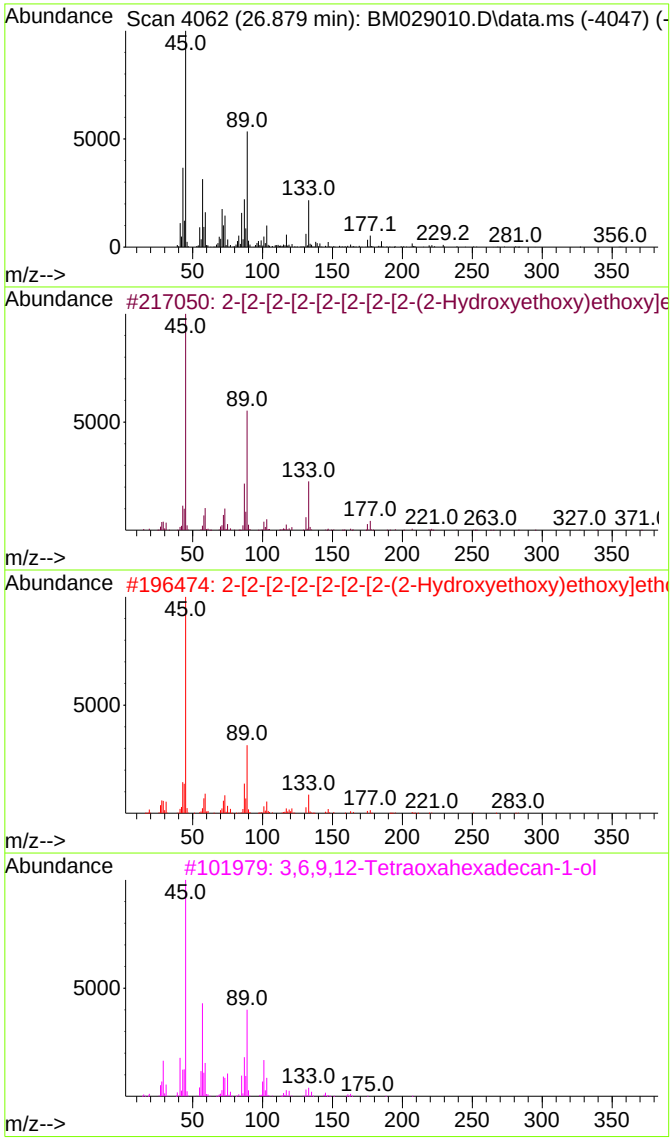
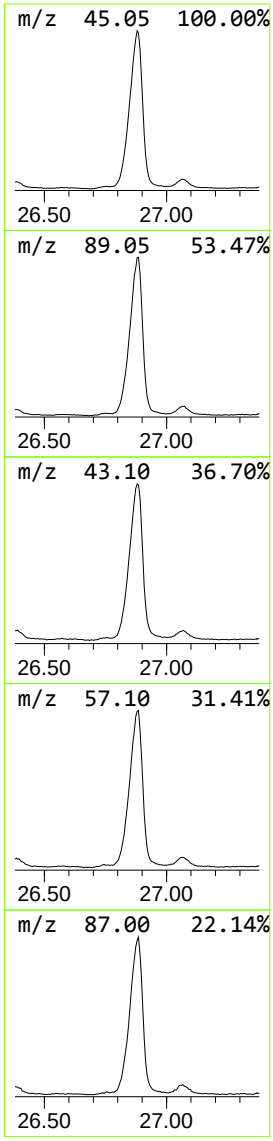
Peak Number 19 3,6,9,12-Tetraoxahexadecan-... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.879	315.56 ng	2626840	Perylene-d12	23.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	91
2	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	91
3	3,6,9,12-Tetraoxahexadecan-1-ol	250	C12H26O5	001559-34-8	86
4	3,6,9,12,15-Pentaoxanonadecan-1-ol	294	C14H30O6	001786-94-3	83
5	2-[2-[2-[2-[2-(2-Methoxyethox...	340	C15H32O8	1000352-04-1	83





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM029010.D
Acq On : 05 Mar 2021 23:46
Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

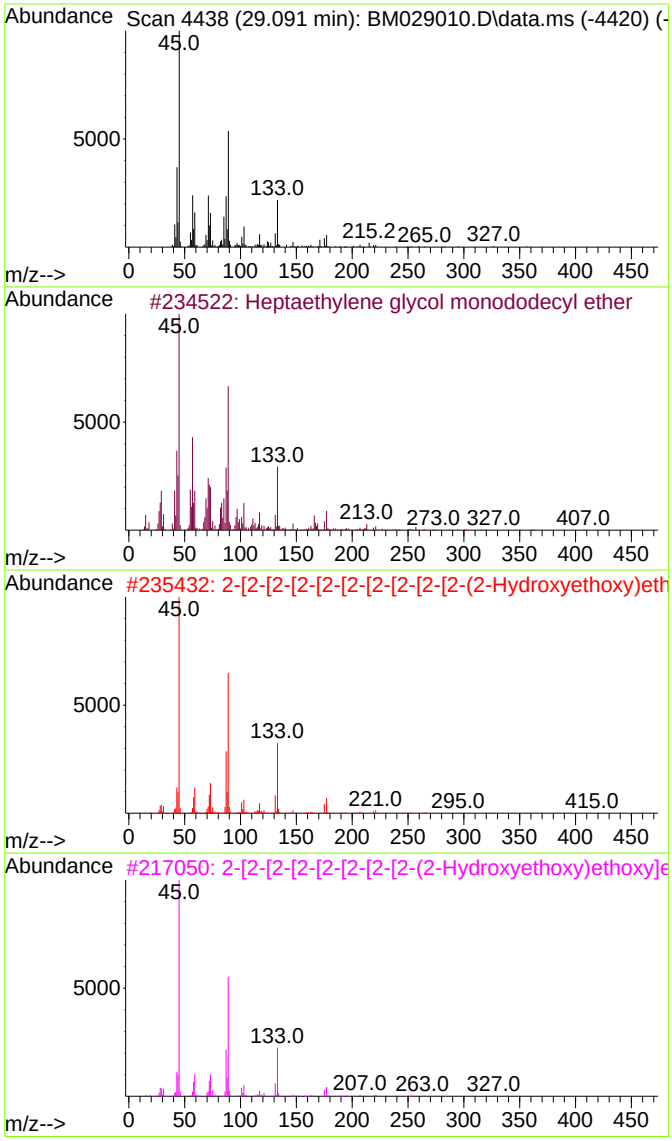
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

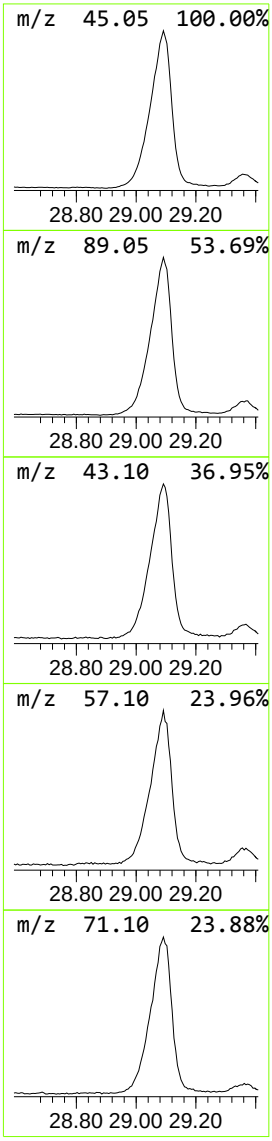
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 Heptaethylene glycol monodo... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.091	213.56 ng	1777750	Perylene-d12	23.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptaethylene glycol monododecyl...	494	C26H54O8	003055-97-8	91
2	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-(2-...	502	C22H46O12	1000352-13-2	87
3	2-[2-[2-[2-[2-[2-[2-[2-(2-Hydrox...	414	C18H38O10	1000352-12-5	87
4	2-[2-[2-[2-[2-[2-[2-[2-[2-[2-[2-...	546	C24H50O13	1000352-12-7	87
5	2-[2-[2-[2-[2-[2-[2-(2-Hydroxyet...	370	C16H34O9	005117-19-1	87





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM030521\
Data File : BM029010.D
Acq On : 05 Mar 2021 23:46
Operator : CG/JU
Sample : M1552-06
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 435-416

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM022321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Oxalic acid, al...	13.321	210.8	ng	1727790	3	14.345	163922	20.0
Methoxyacetic a...	16.015	516.7	ng	3715050	4	17.092	143794	20.0
Diethylene glyc...	16.815	291.6	ng	2096160	4	17.092	143794	20.0
Methoxyacetic a...	17.568	177.6	ng	1277090	4	17.092	143794	20.0
Octaethylene gl...	18.092	772.2	ng	5551660	4	17.092	143794	20.0
Triethylene gly...	18.750	539.4	ng	3877880	4	17.092	143794	20.0
Pentaethylene g...	20.286	350.8	ng	5060710	5	21.268	288490	20.0
Pentaethylene g...	20.762	192.2	ng	2772530	5	21.268	288490	20.0
Hexaethylene gl...	21.103	482.0	ng	6952950	5	21.268	288490	20.0
2-[2-[2-[2-[2-[...	21.533	380.0	ng	5480900	5	21.268	288490	20.0
Hexaethylene gl...	21.950	188.9	ng	2724290	5	21.268	288490	20.0
2-[2-[2-[2-[2-[...	22.291	420.1	ng	6060010	5	21.268	288490	20.0
3,6,9,12,15-Pen...	22.774	567.6	ng	4725140	6	23.433	166490	20.0
Heptaethylene g...	23.309	240.3	ng	2000100	6	23.433	166490	20.0
2-[2-[2-[2-[2-[...	23.756	610.3	ng	5080010	6	23.433	166490	20.0
2-[2-[2-[2-[2-[...	24.433	459.4	ng	3824570	6	23.433	166490	20.0
unknown25.197	25.197	180.9	ng	1505570	6	23.433	166490	20.0
unknown25.862	25.862	409.3	ng	3407090	6	23.433	166490	20.0
3,6,9,12-Tetrao...	26.879	315.6	ng	2626840	6	23.433	166490	20.0
Heptaethylene g...	29.091	213.6	ng	1777750	6	23.433	166490	20.0