LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046356.D
Acq On : 28 Jun 2024 17:23
Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

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-BM062724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM046356.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.681	127	135	147	rVB	414696	665703	8.05%	1.222%
2	5.016	353	362	365	rBV2	79771	178888	2.16%	0.328%
3	5.063	365	370	386	rVB2	208807	465283	5.62%	0.854%
4	5.416	424	430	438	rVB2	225448	396398	4.79%	0.728%
5	5.663	464	472	478	rBV4	62374	145774	1.76%	0.268%
6	5.881	502	509	515	rBV4	65361	131544	1.59%	0.242%
7	5.952	515	521	525	rBV	67853	120579	1.46%	0.221%
8	6.016	525	532	537	rBV3	76580	153144	1.85%	0.281%
9	6.375	581	593	598	rBV5	126884	280280	3.39%	0.515%
10	6.428	598	602	606	rBV	81444	120524	1.46%	0.221%
11	6.475	606	610	616	rVV	186638	298369	3.61%	0.548%
12	6.534	616	620	626	rVB2	160754	270407	3.27%	0.497%
13	6.604	626	632	635	rBV2	87657	141216	1.71%	0.259%
14	6.646	635	639	644	rVB	86035	137309	1.66%	0.252%
15	6.769	652	660	665	rBV2	78058	158840	1.92%	0.292%
16	6.999	693	699	701	rBV	371979	562082	6.80%	1.032%
17	7.269	738	745	752	rBV5	49500	146673	1.77%	0.269%
18	7.369	752	762	767	rBV2	701790	1203029	14.54%	2.209%
19	7.475	775	780	789	rBV4	142419	277110	3.35%	0.509%
20	7.634	802	807	815	rBV5	83199	181778	2.20%	0.334%
21	7.734	816	824	831	rVB2	72636	179643	2.17%	0.330%
22	7.857	840	845	848	rBV3	77080	128588	1.55%	0.236%
23	7.904	848	853	858	rVB2	153186	300368	3.63%	0.552%
24	8.004	865	870	877	rBV3	164987	321539	3.89%	0.590%
25	8.128	883	891	893	rBV3	90849	154746	1.87%	0.284%
26	8.163	893	897	902	rVB	132156	198895	2.40%	0.365%
27	8.310	917	922	927	rBV	77386	141563	1.71%	0.260%
28	8.363	927	931	936	rVB	65829	98273	1.19%	0.180%
29	8.457	943	947	955	rVB	150923	234299	2.83%	0.430%
30	8.540	955	961	965	rBV3	158939	295054	3.57%	0.542%
31	8.587	965	969	976	rVB	393271	571147	6.90%	1.049%
32	8.704	978	989	994	rBV10	81997	210152	2.54%	0.386%
33	8.916	994	1025	1028	rBV	1371174	7582144	91.66%	13.923%
34	9.040	1041	1046	1051	rVV2	164720	264429	3.20%	0.486%
35	9.098	1051	1056	1063	rVB	430813	646719	7.82%	1.188%
36	9.245	1075	1081	1086	rBV4	53915	144119	1.74%	0.265%

LSC Area Percent Report

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Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

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-BM062724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	9.298	1086	1090	1094	rVB3	71192	112660	1.36%	0.207%
38	9.498	1120	1124	1126	rBV2	84916	114073	1.38%	0.209%
39	9.534	1126	1130	1134	rVB2	112798	166739	2.02%	0.306%
40	9.581	1134	1138	1141	rBV2	102324	142243	1.72%	0.261%
41	9.687	1151	1156	1159	rBV3	57786	111592	1.35%	0.205%
42	9.763	1165	1169	1174	rVB	118409	195448	2.36%	0.359%
43	9.981	1201	1206	1211	rBV3	61000	126083	1.52%	0.232%
44	10.128	1224	1231	1237	rVV2	960522	1760875	21.29%	3.234%
45	10.181	1237	1240	1247	rVV5	59481	109685	1.33%	0.201%
46	10.245	1247	1251	1257	rVB3	72316	127528	1.54%	0.234%
47	10.304	1257	1261	1265	rBV	69396	95084	1.15%	0.175%
48	10.592	1305	1310	1318	rVB5	58319	120890	1.46%	0.222%
49	10.698	1322	1328	1334	rBV	612429	959120	11.60%	1.761%
50	10.763	1334	1339	1352	rVB	553055	1116555	13.50%	2.050%
51	11.039	1380	1386	1394	rBV4	81221	167418	2.02%	0.307%
52	11.145	1399	1404	1408	rBV2	61090	100093	1.21%	0.184%
53	11.310	1425	1432	1440	rBV3	102384	181583	2.20%	0.333%
54	11.563	1469	1475	1484	rVB	191586	306823	3.71%	0.563%
55	11.763	1503	1509	1523	rVB	2596649	3943409	47.67%	7.241%
56	11.934	1533	1538	1546	rBV	115981	240760	2.91%	0.442%
57	12.051	1555	1558	1566	rVB3	59243	106897	1.29%	0.196%
58	12.551	1639	1643	1652	rVB3	70734	105830	1.28%	0.194%
59	12.633	1652	1657	1661	rBV	249065	391555	4.73%	0.719%
60	12.845	1684	1693	1700	rBV	224466	364545	4.41%	0.669%
61	13.833	1857	1861	1866	rVB	61276	90836	1.10%	0.167%
62	13.939	1873	1879	1884	rBV	241113	334944	4.05%	0.615%
63	14.016	1886	1892	1908	rVV	1070130	1751130	21.17%	3.216%
64	14.286	1935	1938	1947	rVB	62222	107957	1.31%	0.198%
65	14.392	1949	1956	1963	rBV	897614	1520926	18.39%	2.793%
66	14.563	1981	1985	1993	rVB2	61661	104588	1.26%	0.192%
67	14.822	2022	2029	2038	rBV	1099432	1986769	24.02%	3.648%
68	14.898	2038	2042	2051	rVB	176270	271241	3.28%	0.498%
69	15.533	2142	2150	2154	rBV7	60193	115621	1.40%	0.212%
70	15.763	2185	2189	2191	rBV	75112	104985	1.27%	0.193%
71	16.027	2230	2234	2241	rVB2	69089	91477	1.11%	0.168%
72	16.098	2241	2246	2249	rBV2	58528	93779	1.13%	0.172%
73	16.133	2249	2252	2255	rVV	110794	122790	1.48%	0.225%
74	16.251	2268	2272	2277	rVB2	81901	121338	1.47%	0.223%
75	16.321	2279	2284	2288	rBV4	58733	91008	1.10%	0.167%
76	16.774	2355	2361	2372	rBV	1100616	1612496	19.49%	2.961%

LSC Area Percent Report

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Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

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

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Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

77	17.392	2462	2466	2471	rBV	183981	243863	2.95%	0.448%
78	17.468	2475	2479	2489	rVB4	64746	119871	1.45%	0.220%
79	17.704	2509	2519	2527	rBV3	245677	688740	8.33%	1.265%
80	17.974	2561	2565	2574	rVB3	62006	135591	1.64%	0.249%
81	18.774	2697	2701	2706	rBV	95861	125646	1.52%	0.231%
82	18.886	2715	2720	2727	rVB	1786614	1962054	23.72%	3.603%
83	18.992	2735	2738	2739	rBV	114665	121600	1.47%	0.223%
84	19.015	2739	2742	2749	rVB	187000	290102	3.51%	0.533%
85	19.110	2754	2758	2762	rVB2	163109	201082	2.43%	0.369%
86	19.198	2770	2773	2778	rVV	81860	116000	1.40%	0.213%
87	19.245	2778	2781	2787	rVB	97124	139847	1.69%	0.257%
88	19.339	2792	2797	2805	rBV	7922092	8271780	100.00%	15.190%
89	19.421	2807	2811	2818	rVB	295854	426850	5.16%	0.784%
90	19.745	2862	2866	2870	rBV	164608	216206	2.61%	0.397%
91	19.933	2895	2898	2907	rVB	92901	138144	1.67%	0.254%
92	20.133	2929	2932	2935	rBV	166240	189485	2.29%	0.348%
93	20.239	2947	2950	2953	rBV	125463	139539	1.69%	0.256%
94	20.704	3026	3029	3032	rBV	140595	145067	1.75%	0.266%
95	20.992	3073	3078	3089	rVB	852775	1262742	15.27%	2.319%
96	21.115	3096	3099	3102	rBV	146627	151501	1.83%	0.278%
97	21.539	3167	3171	3181	rVB	202139	285769	3.45%	0.525%
98	21.674	3191	3194	3199	rVB	137640	172232	2.08%	0.316%
99	22.233	3285	3289	3294	rVB	185720	271579	3.28%	0.499%
100	23.662	3526	3532	3543	rVB	557464	1445472	17.47%	2.654%

Sum of corrected areas: 54456743

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
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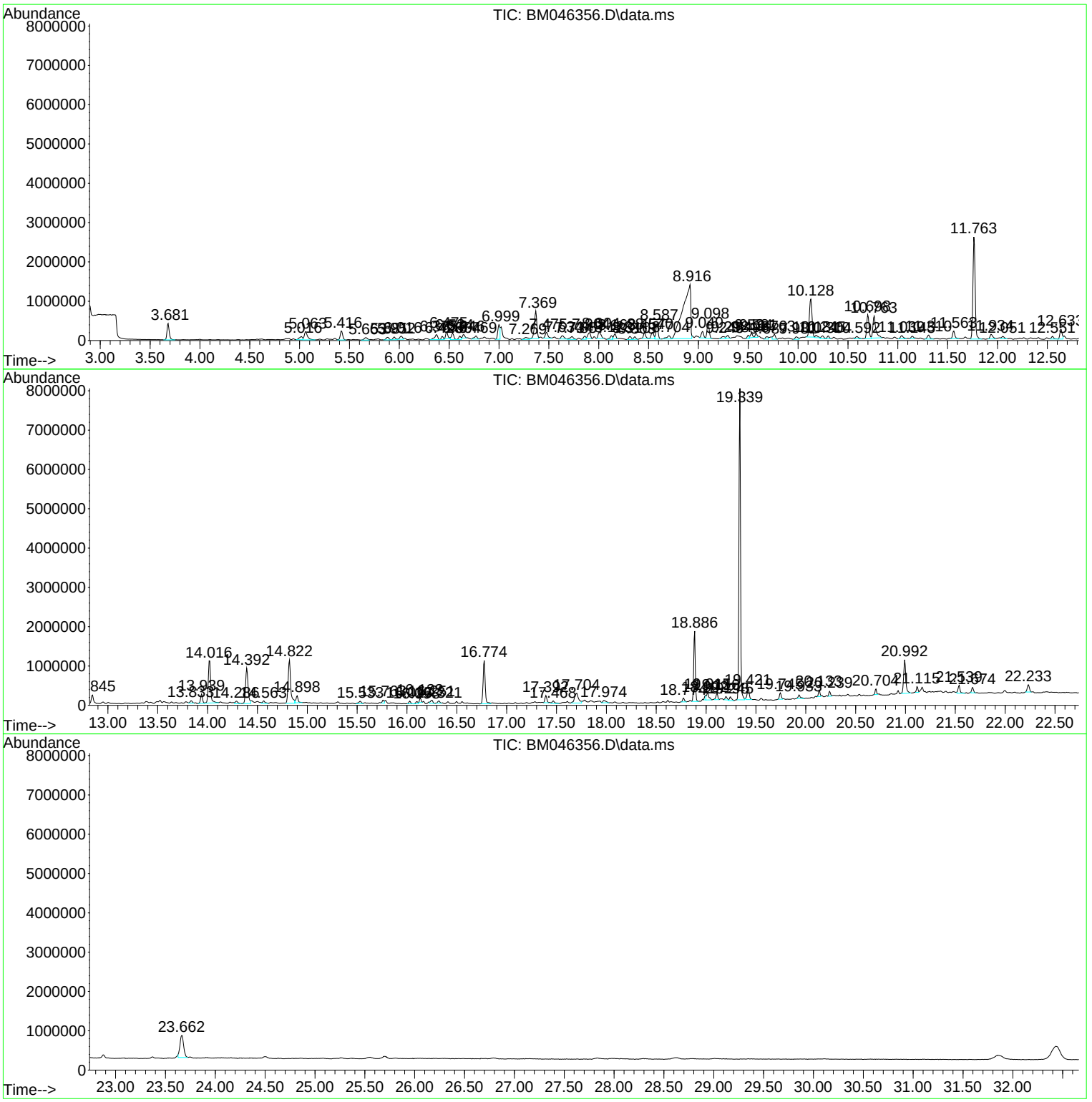
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046356.D
Acq On : 28 Jun 2024 17:23
Operator : MA/JU
Sample : P3049-01 10X
Misc :
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Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

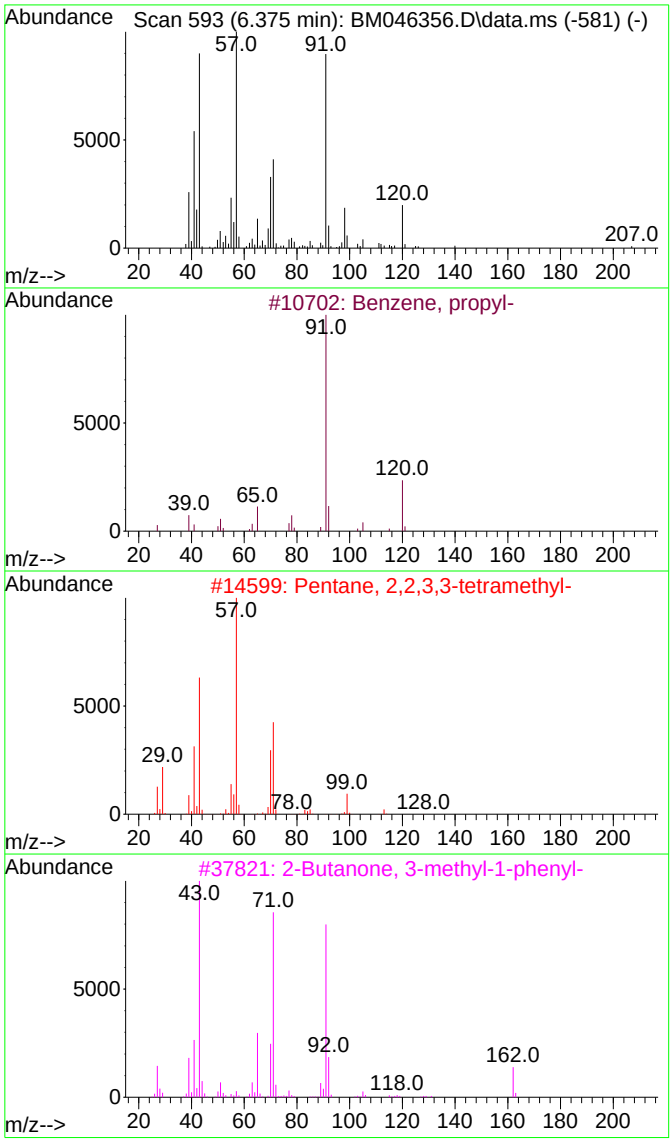
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

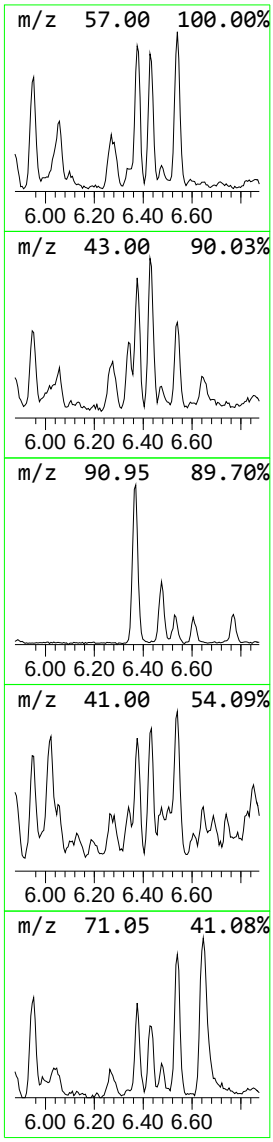
****

Peak Number 3 unknown6.375 Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.375	4.66 ng	280280	1,4-Dichlorobenzene-d4	7.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, propyl-	120	C9H12	000103-65-1	38
2	Pentane, 2,2,3,3-tetramethyl-	128	C9H20	007154-79-2	38
3	2-Butanone, 3-methyl-1-phenyl-	162	C11H14O	002893-05-2	27
4	Sulfurous acid, 2-ethylhexyl und...	348	C19H40O3S	1000309-19-4	27
5	Benzene, (ethenyloxy)-	120	C8H8O	000766-94-9	22





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046356.D
Acq On : 28 Jun 2024 17:23
Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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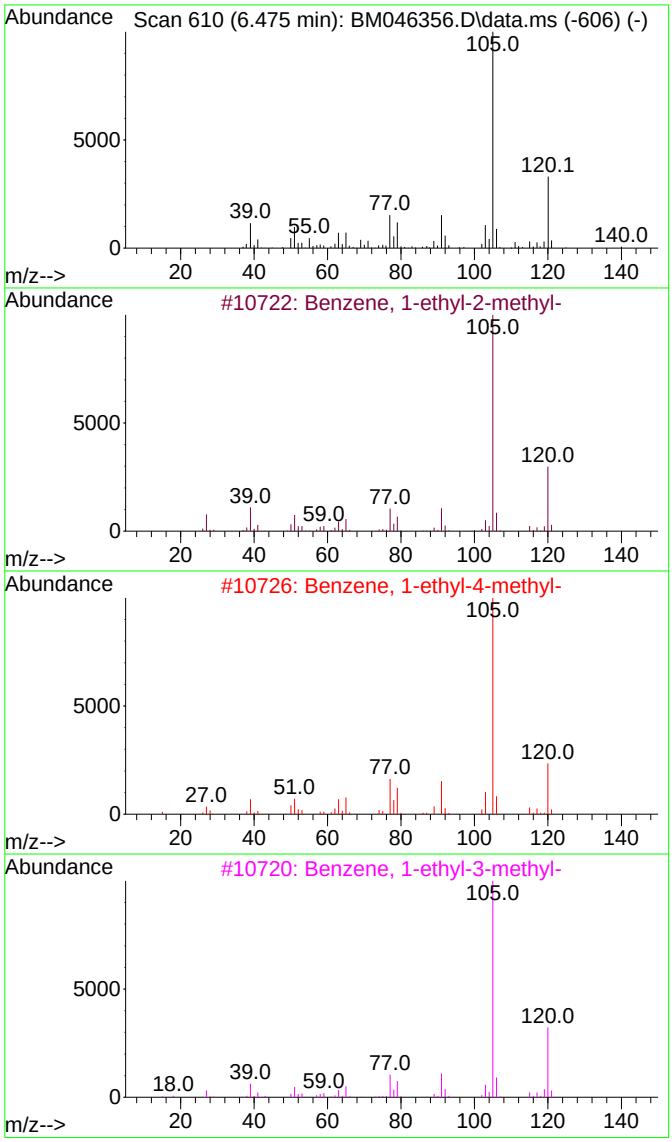
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

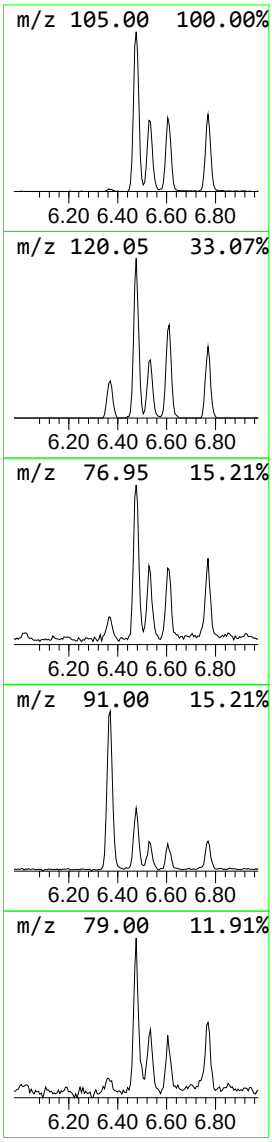
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Benzene, 1-ethyl-2-methyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.475	4.96 ng	298369	1,4-Dichlorobenzene-d4	7.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3	Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
4	Mesitylene	120	C9H12	000108-67-8	91
5	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046356.D
Acq On : 28 Jun 2024 17:23
Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

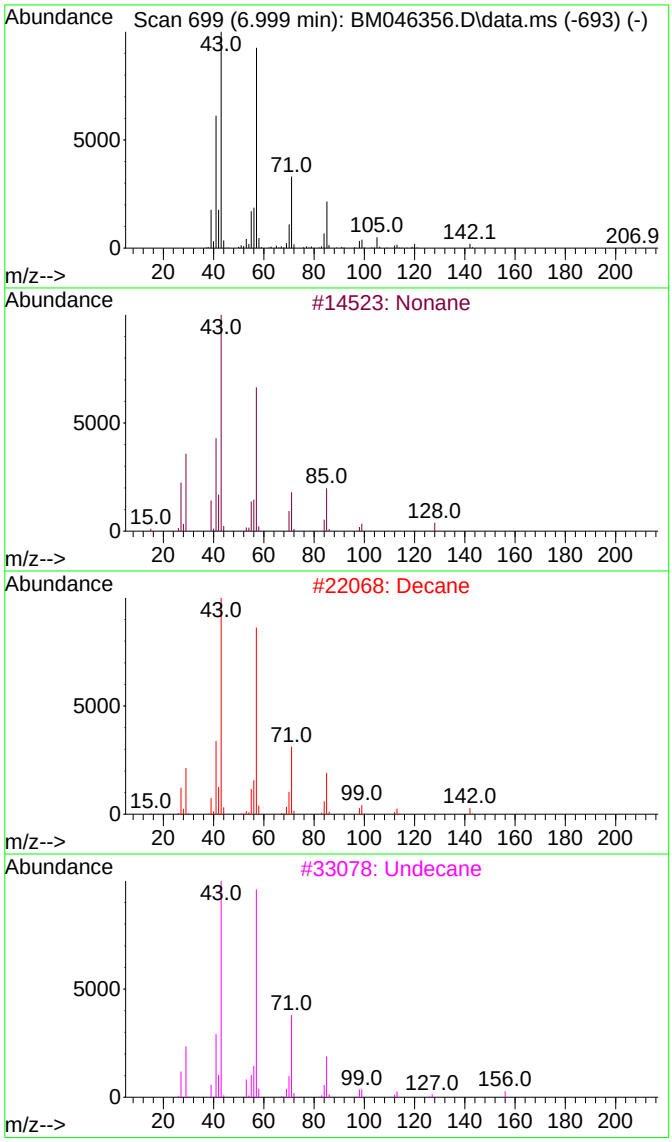
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

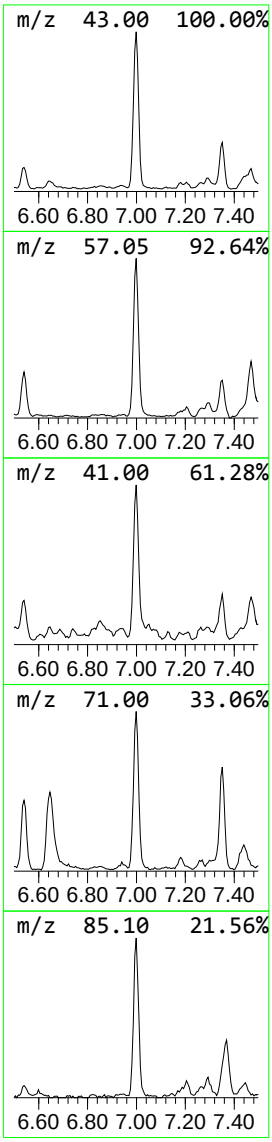
****

Peak Number 5 Nonane Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.999	9.34 ng	562082	1,4-Dichlorobenzene-d4	7.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonane	128	C9H20	000111-84-2	86
2	Decane	142	C10H22	000124-18-5	83
3	Undecane	156	C11H24	001120-21-4	83
4	Carbonic acid, prop-1-en-2-yl tr...	284	C17H32O3	1000382-90-8	72
5	Tridecane	184	C13H28	000629-50-5	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046356.D
Acq On : 28 Jun 2024 17:23
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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

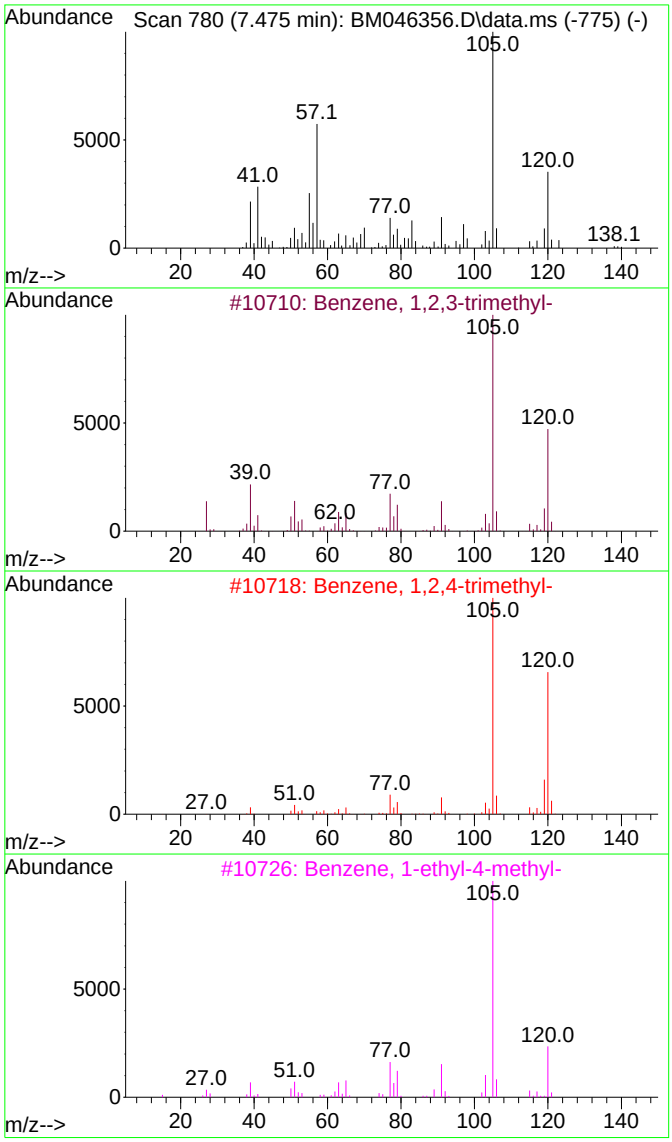
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

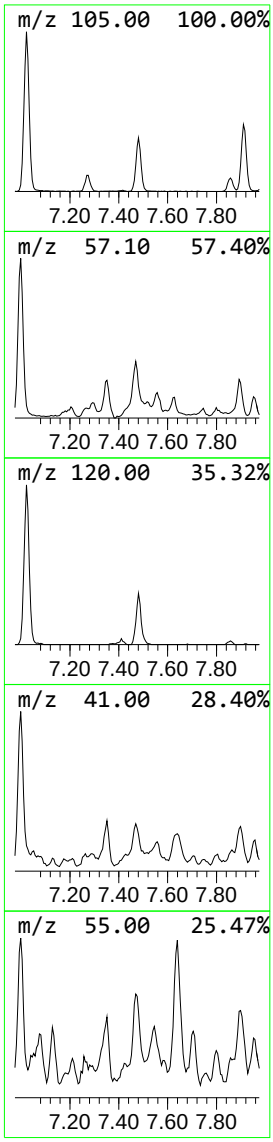
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 6 Benzene, 1,2,3-trimethyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.475	4.61 ng	277110	1,4-Dichlorobenzene-d4	7.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	94
2	Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	93
3	Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4	Mesitylene	120	C9H12	000108-67-8	87
5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	76





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046356.D
Acq On : 28 Jun 2024 17:23
Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

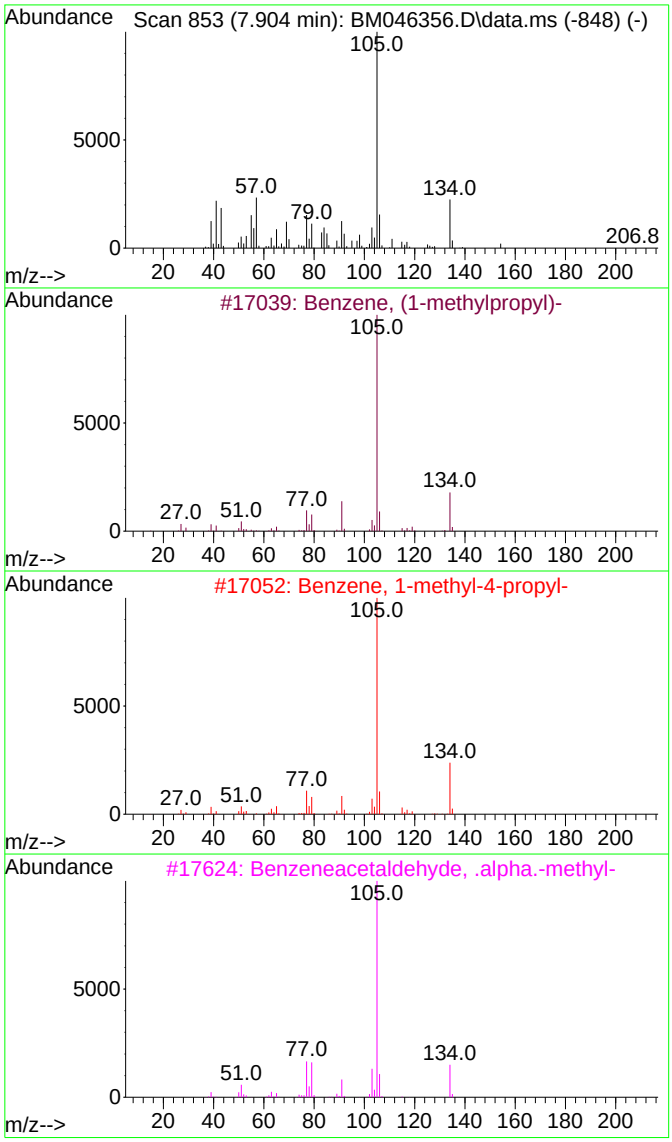
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

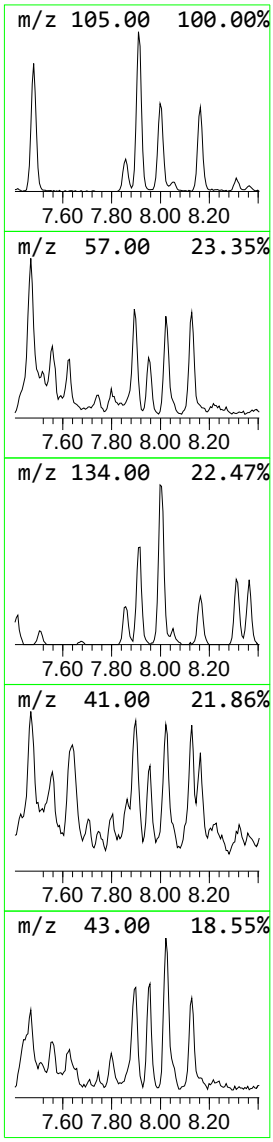
****

Peak Number 7 Benzene, (1-methylpropyl)- Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.904	4.99 ng	300368	1,4-Dichlorobenzene-d4	7.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, (1-methylpropyl)-	134	C10H14	000135-98-8	70
2	Benzene, 1-methyl-4-propyl-	134	C10H14	001074-55-1	70
3	Benzeneacetaldehyde, .alpha.-met...	134	C9H10O	000093-53-8	70
4	2-Tolyloxirane	134	C9H10O	002783-26-8	70
5	Benzene, 1-methyl-3-propyl-	134	C10H14	001074-43-7	64





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Data File : BM046356.D
Acq On : 28 Jun 2024 17:23
Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

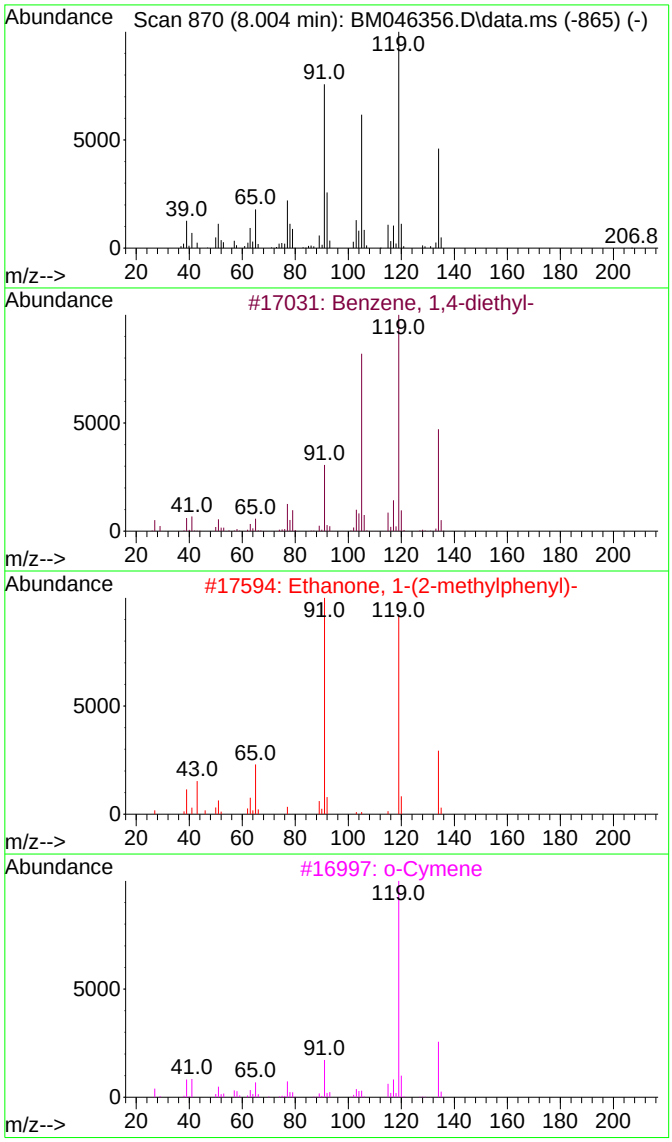
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

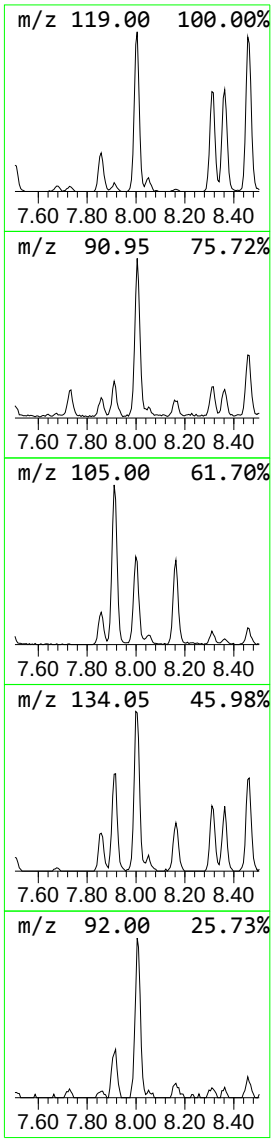
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 8 Benzene, 1,4-diethyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.004	5.35 ng	321539	1,4-Dichlorobenzene-d4	7.369

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzene, 1,4-diethyl-	134	C10H14	000105-05-5	93
2	Ethanone, 1-(2-methylphenyl)-	134	C9H10O	000577-16-2	92
3	o-Cymene	134	C10H14	000527-84-4	91
4	Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	90
5	Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	90





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Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

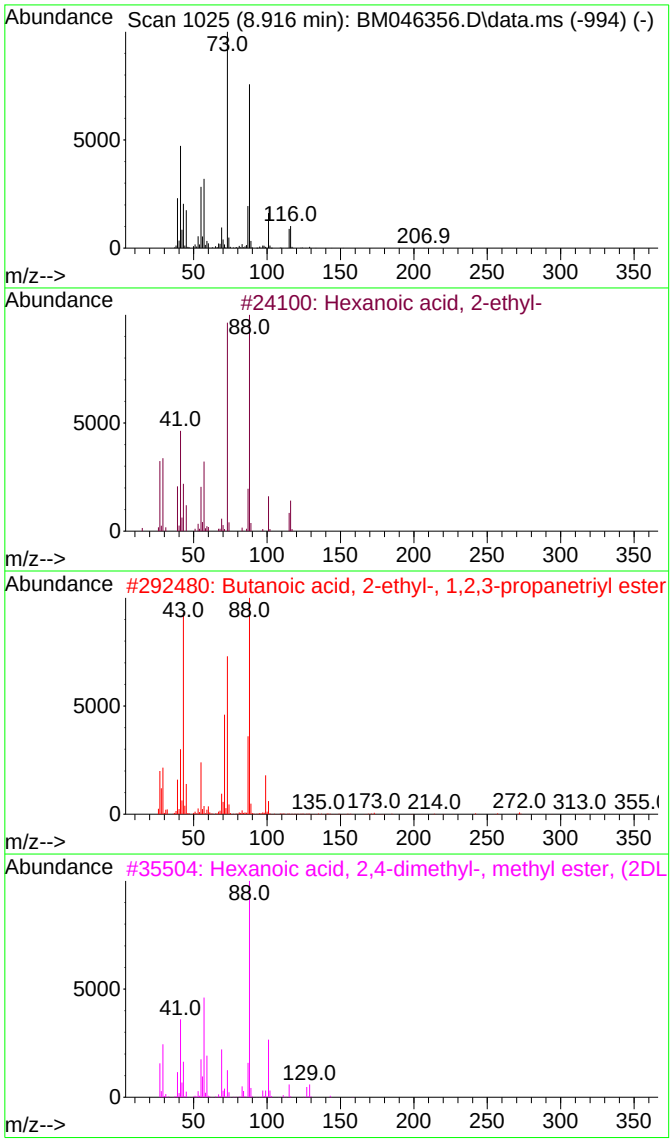
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

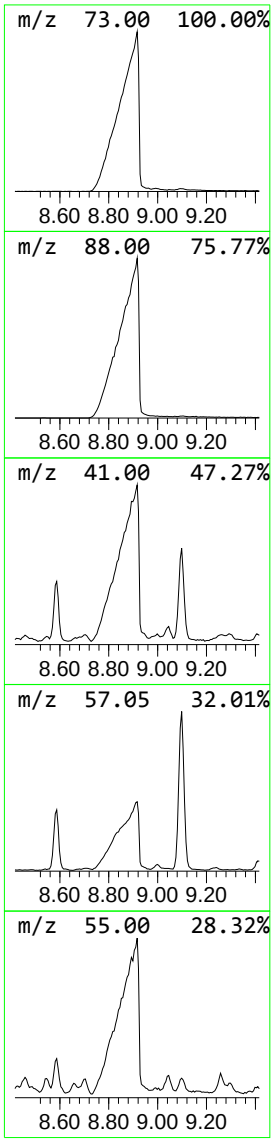
****

Peak Number 9 Hexanoic acid, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.916	86.12 ng	7582140	Naphthalene-d8	10.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	90
2	Butanoic acid, 2-ethyl-, 1,2,3-p...	386	C21H38O6	056554-54-2	59
3	Hexanoic acid, 2,4-dimethyl-, me...	158	C9H18O2	014251-44-6	53
4	Pentanoic acid, 2,4-dimethyl-, m...	144	C8H16O2	071672-33-8	40
5	Cyclohexaneacetic acid, .alpha.-...	170	C10H18O2	006051-00-9	40





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Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

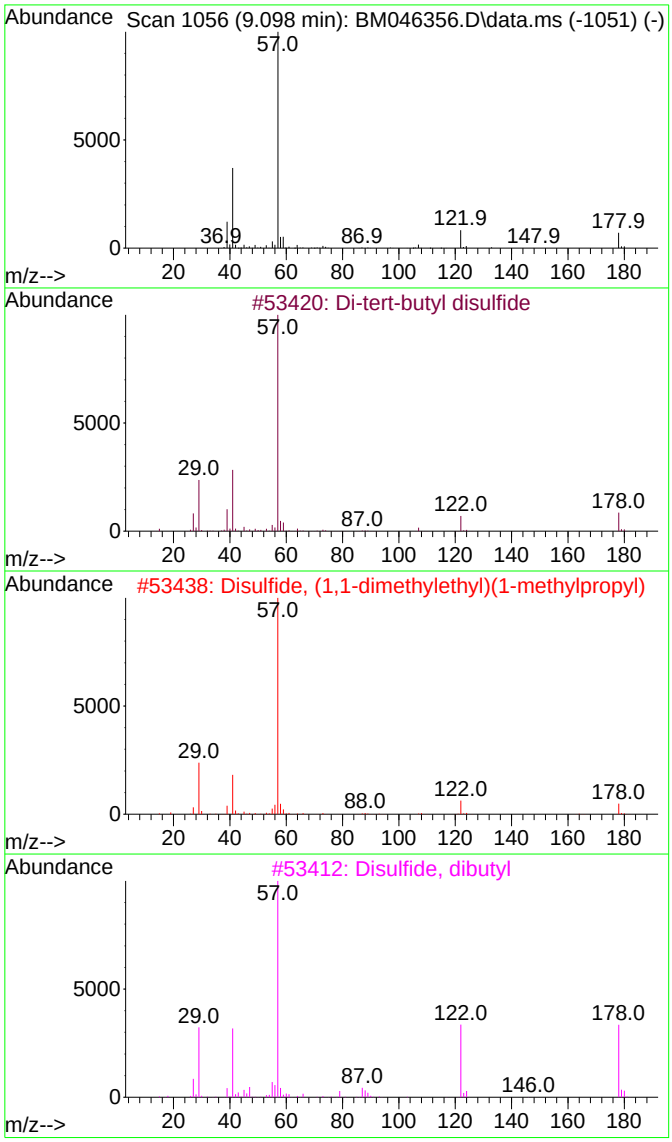
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

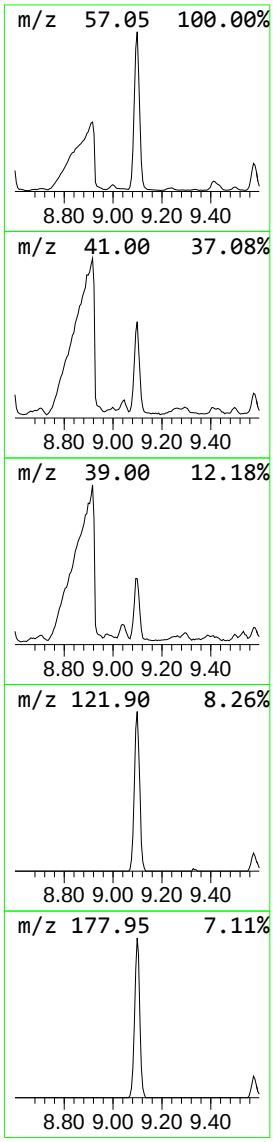
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 10 Di-tert-butyl disulfide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.098	7.35 ng	646719	Naphthalene-d8	10.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	91
2	Disulfide, (1,1-dimethylethyl)(1...	178	C8H18S2	072437-46-8	64
3	Disulfide, dibutyl	178	C8H18S2	000629-45-8	49
4	Disulfide, bis(1-methylpropyl)	178	C8H18S2	005943-30-6	45
5	Disulfide, (1-methylethyl) (1,1-...	164	C7H16S2	043022-60-2	33





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Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

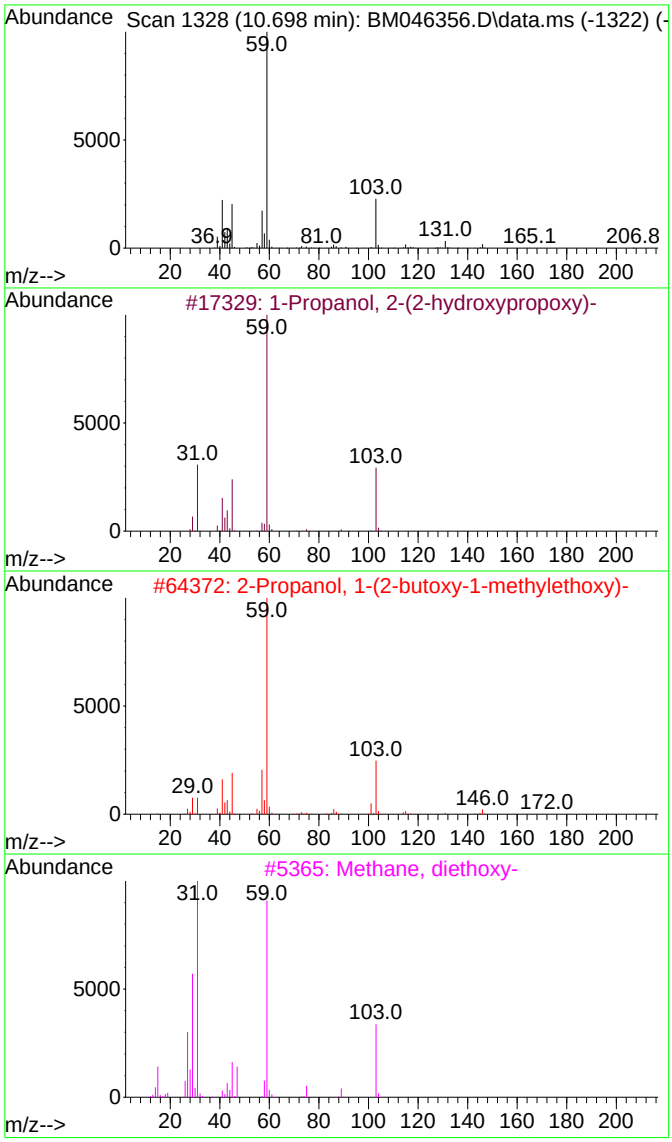
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

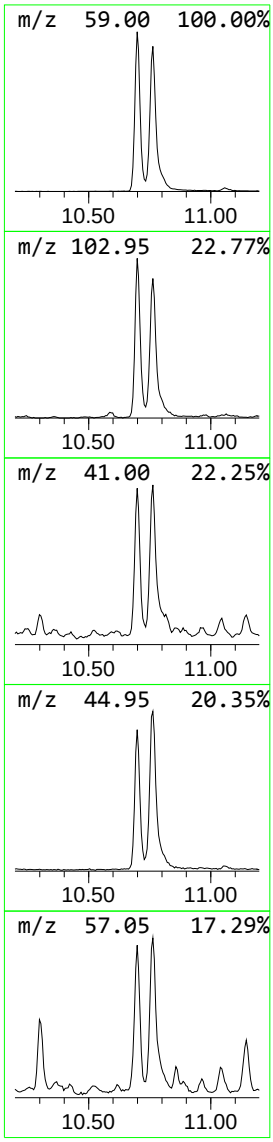
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 11 1-Propanol, 2-(2-hydroxypro... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.698	10.89 ng	959120	Naphthalene-d8	10.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
2	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	78
3	Methane, diethoxy-	104	C5H12O2	000462-95-3	72
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64





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Acq On : 28 Jun 2024 17:23
Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SHOP-RAG-DRUM

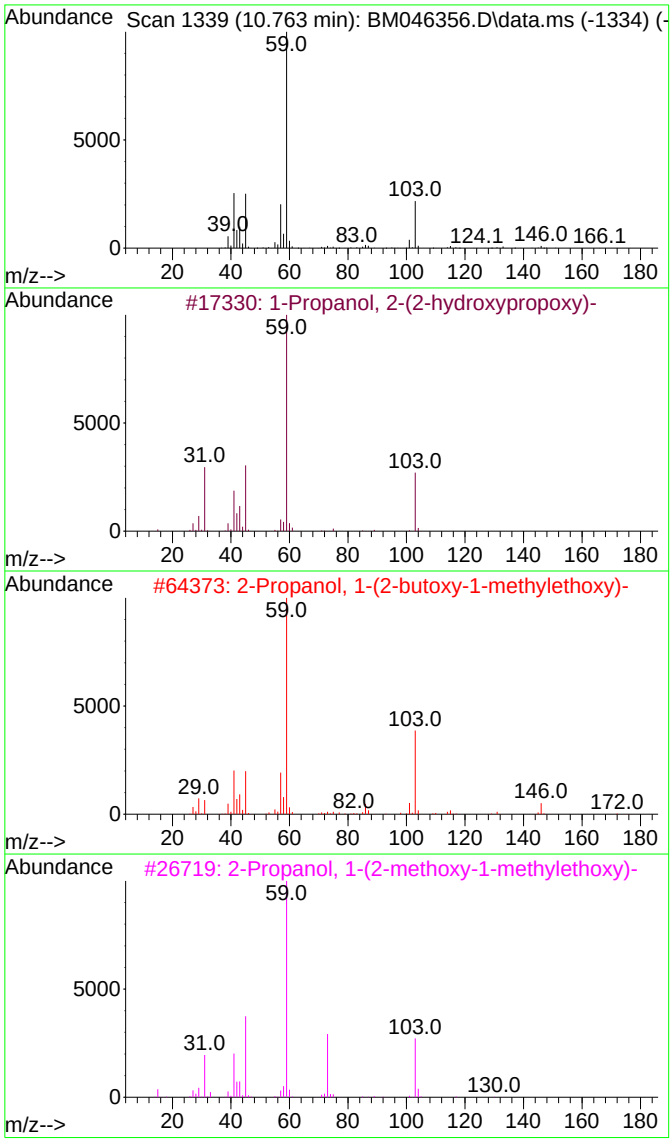
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

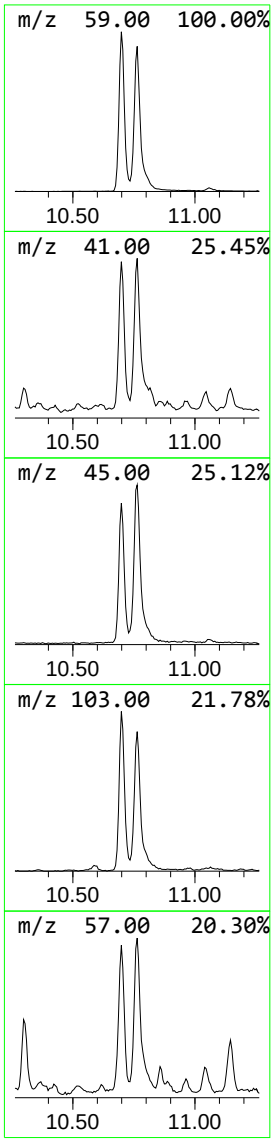
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 12 2-Propanol, 1-(2-butoxy-1-m... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.763	12.68 ng	1116560	Naphthalene-d8	10.128

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Propanol, 2-(2-hydroxypropoxy)-	134	C6H14O3	000106-62-7	78
2	2-Propanol, 1-(2-butoxy-1-methyl...	190	C10H22O3	029911-28-2	74
3	2-Propanol, 1-(2-methoxy-1-methy...	148	C7H16O3	020324-32-7	72
4	1-Propanol, 2,2'-oxybis-	134	C6H14O3	000108-61-2	64
5	Dipropylene glycol (isomer 3)	134	C6H14O3	1000506-25-5	64





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Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SHOP-RAG-DRUM

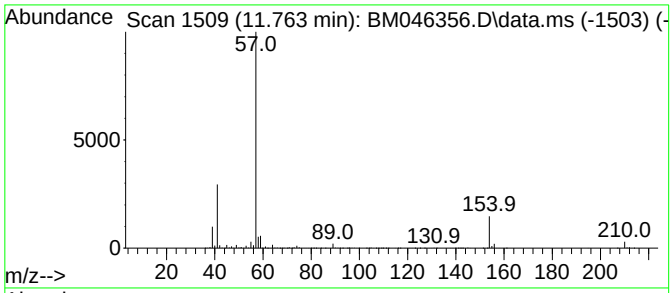
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

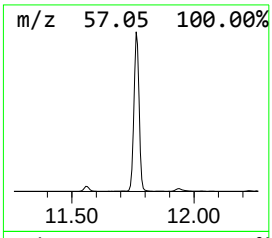
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

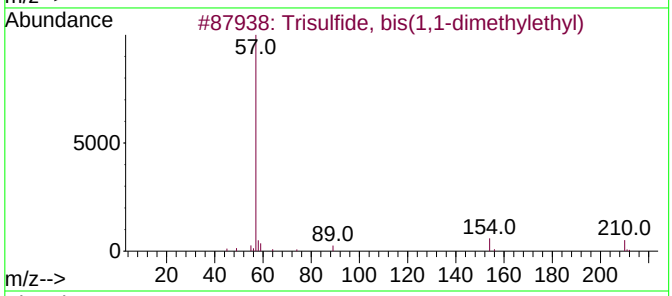
****
Peak Number 13 Trisulfide, bis(1,1-dimethy... Concentration Rank 3

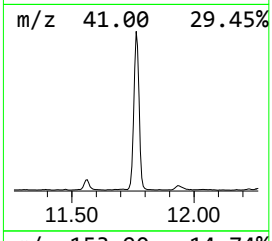
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.763	44.79 ng	3943410	Naphthalene-d8	10.128

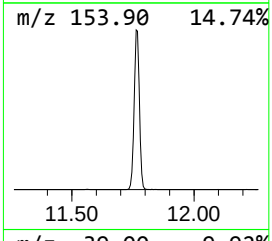
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trisulfide, bis(1,1-dimethylethyl)	210	C8H18S3	004253-90-1	80
2	Di-tert-butyl disulfide	178	C8H18S2	000110-06-5	47
3	di-tert-Butyl dicarbonate	218	C10H18O5	024424-99-5	25
4	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	9
5	Propanoic acid, 2,2-dimethyl-, m...	116	C6H12O2	000598-98-1	9

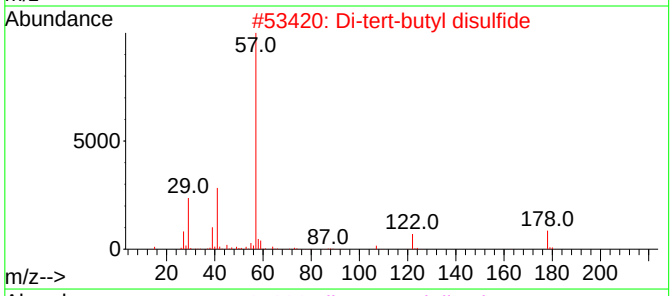


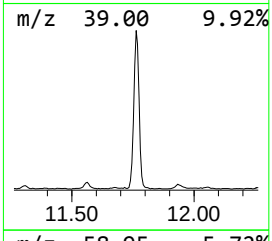


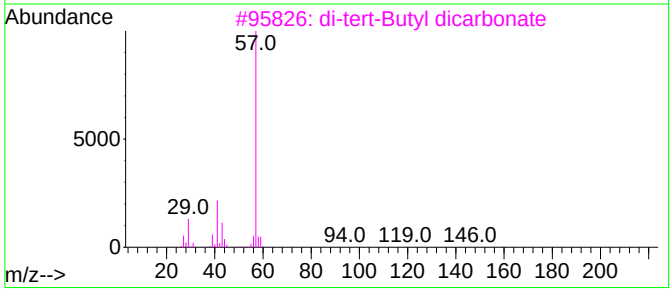


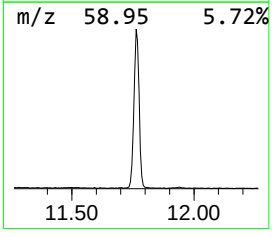












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Acq On : 28 Jun 2024 17:23
Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

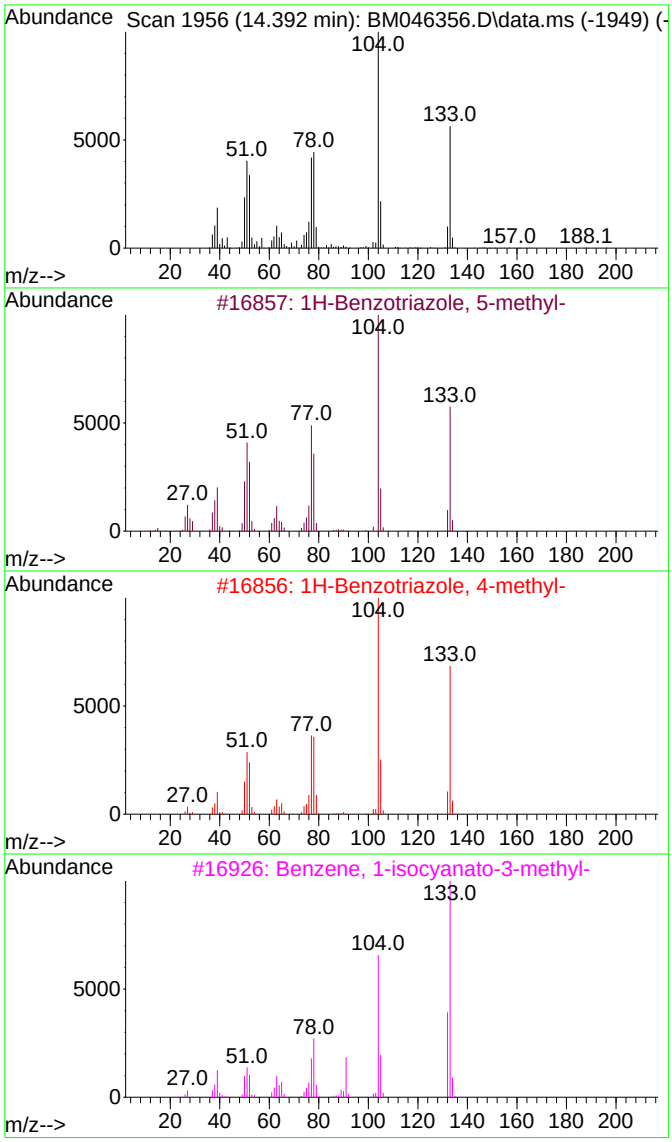
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

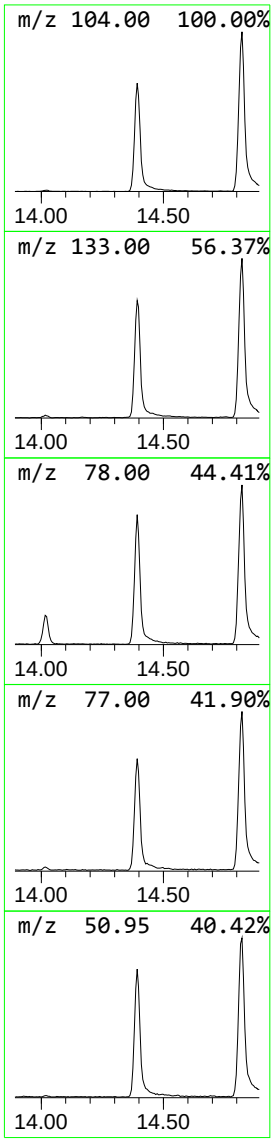
****

Peak Number 14 1H-Benzotriazole, 5-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.392	17.37 ng	1520930	Acenaphthene-d10	14.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	98
2	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	96
3	Benzene, 1-isocyanato-3-methyl-	133	C8H7NO	000621-29-4	90
4	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	87
5	Styrene	104	C8H8	000100-42-5	64





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Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

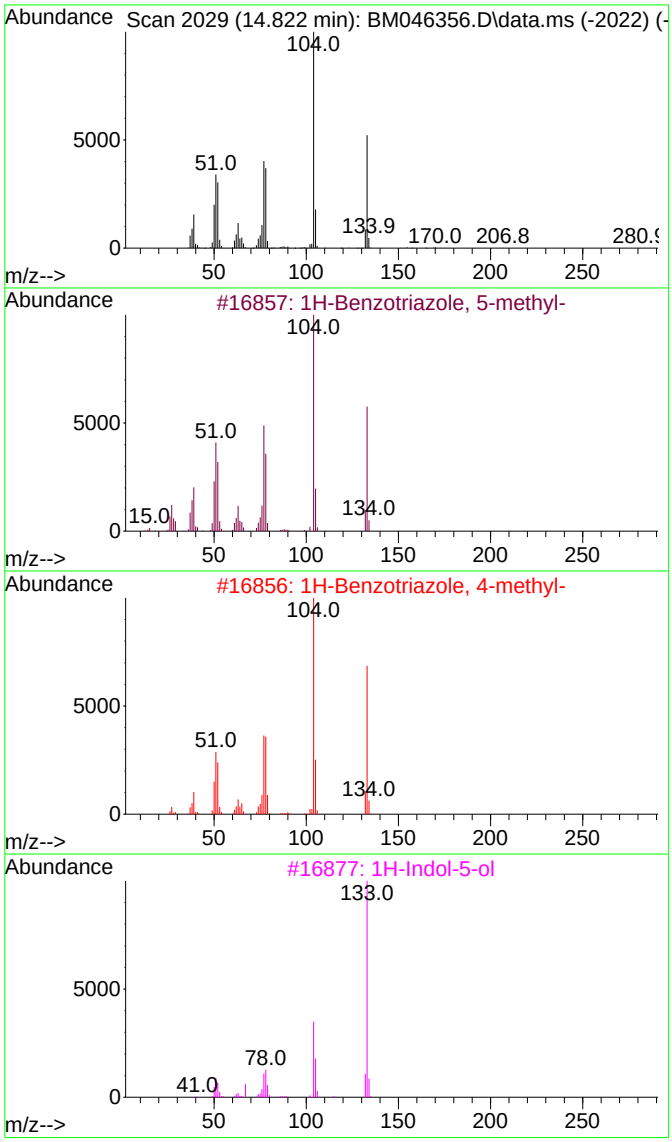
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

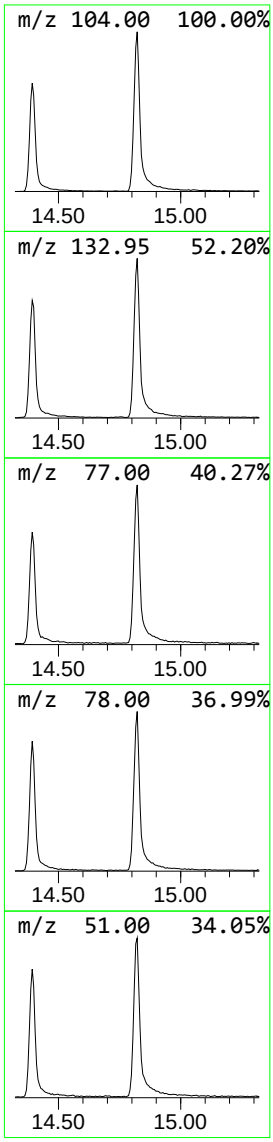
****

Peak Number 15 1H-Benzotriazole, 4-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.822	22.69 ng	1986770	Acenaphthene-d10	14.016

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1H-Benzotriazole, 5-methyl-	133	C7H7N3	000136-85-6	98
2	1H-Benzotriazole, 4-methyl-	133	C7H7N3	029878-31-7	94
3	1H-Indol-5-ol	133	C8H7NO	001953-54-4	91
4	2H-Indol-2-one, 1,3-dihydro-	133	C8H7NO	000059-48-3	83
5	Benzene, 1-azido-2-methyl-	133	C7H7N3	031656-92-5	80





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

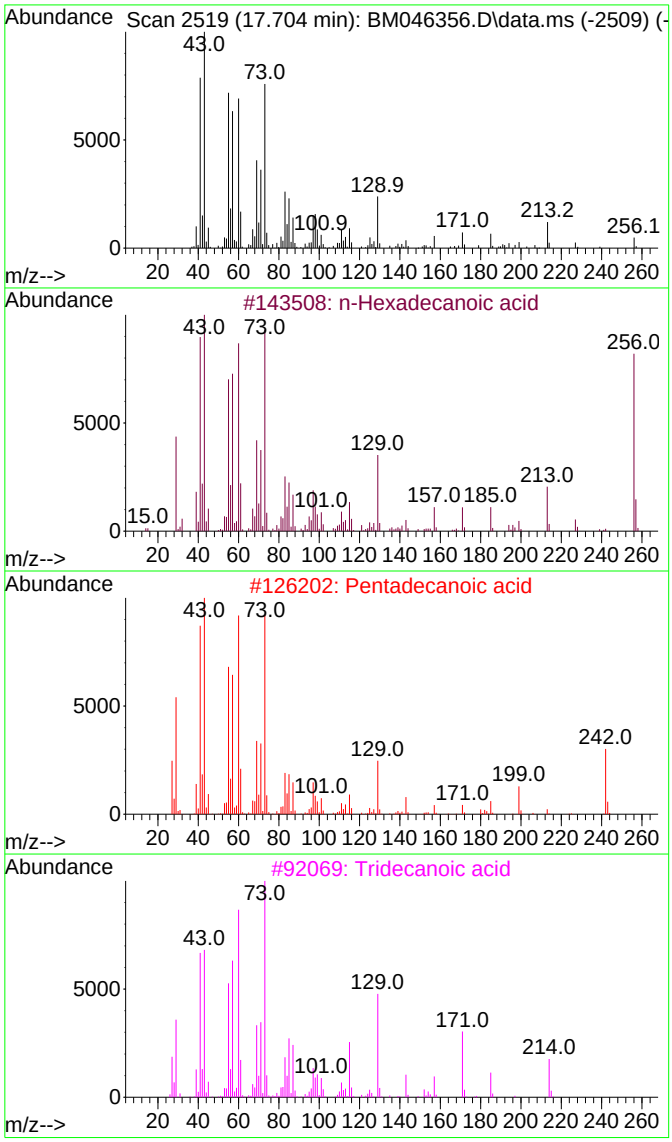
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

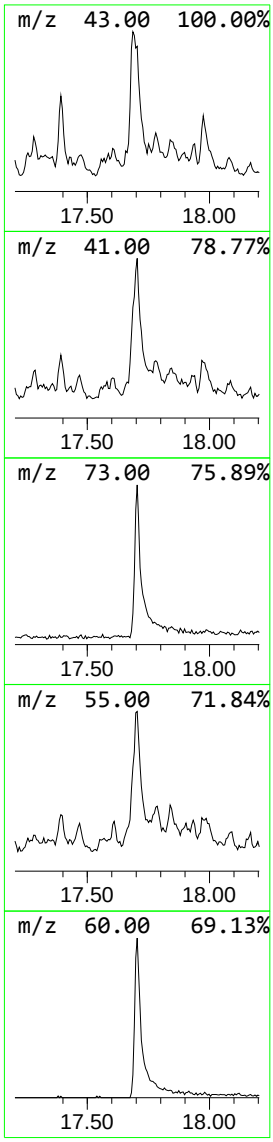
****

Peak Number 16 n-Hexadecanoic acid Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.704	8.54 ng	688740	Phenanthrene-d10	16.774

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3	Tridecanoic acid	214	C13H26O2	000638-53-9	62
4	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46
5	Hexadecyl nonyl ether	368	C25H52O	1000406-37-7	30





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Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

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ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

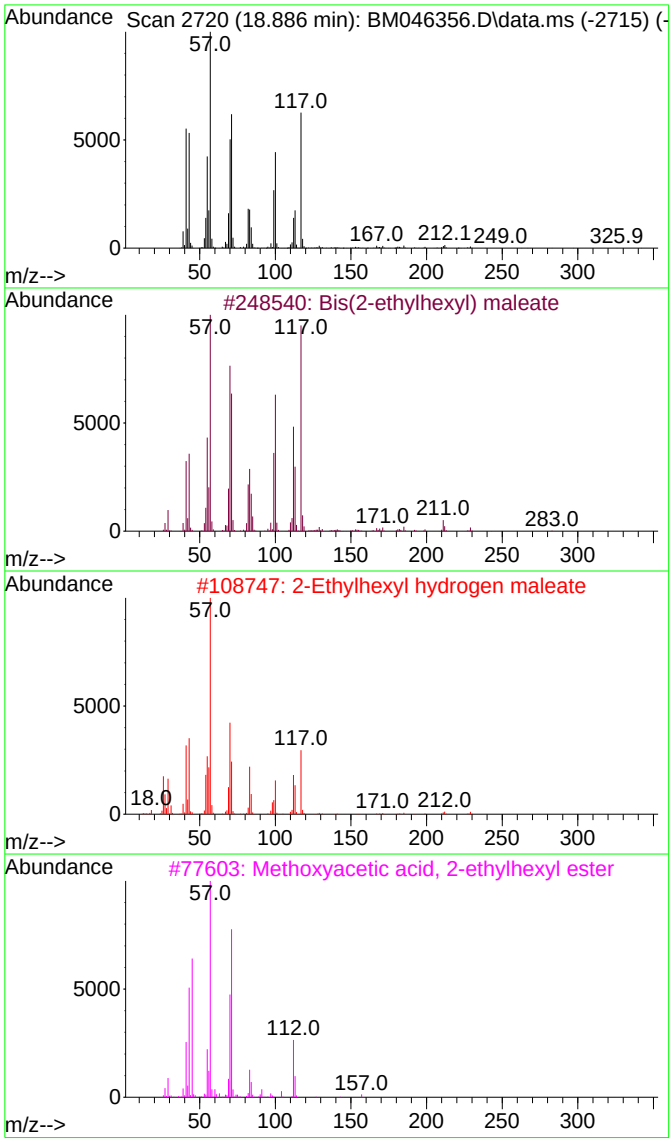
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

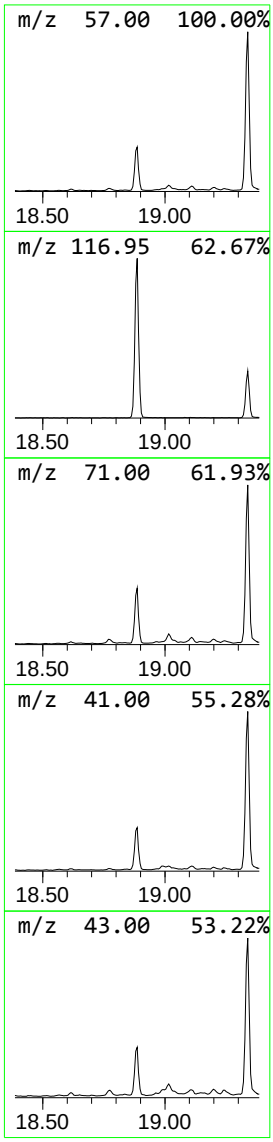
****

Peak Number 17 Bis(2-ethylhexyl) maleate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.886	31.08 ng	1962050	Chrysene-d12	20.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bis(2-ethylhexyl) maleate	340	C20H36O4	000142-16-5	72
2	2-Ethylhexyl hydrogen maleate	228	C12H20O4	002370-71-0	42
3	Methoxyacetic acid, 2-ethylhexyl...	202	C11H22O3	1000282-41-4	38
4	Undecane, 4,5-dimethyl-	184	C13H28	017312-79-7	38
5	Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046356.D
Acq On : 28 Jun 2024 17:23
Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

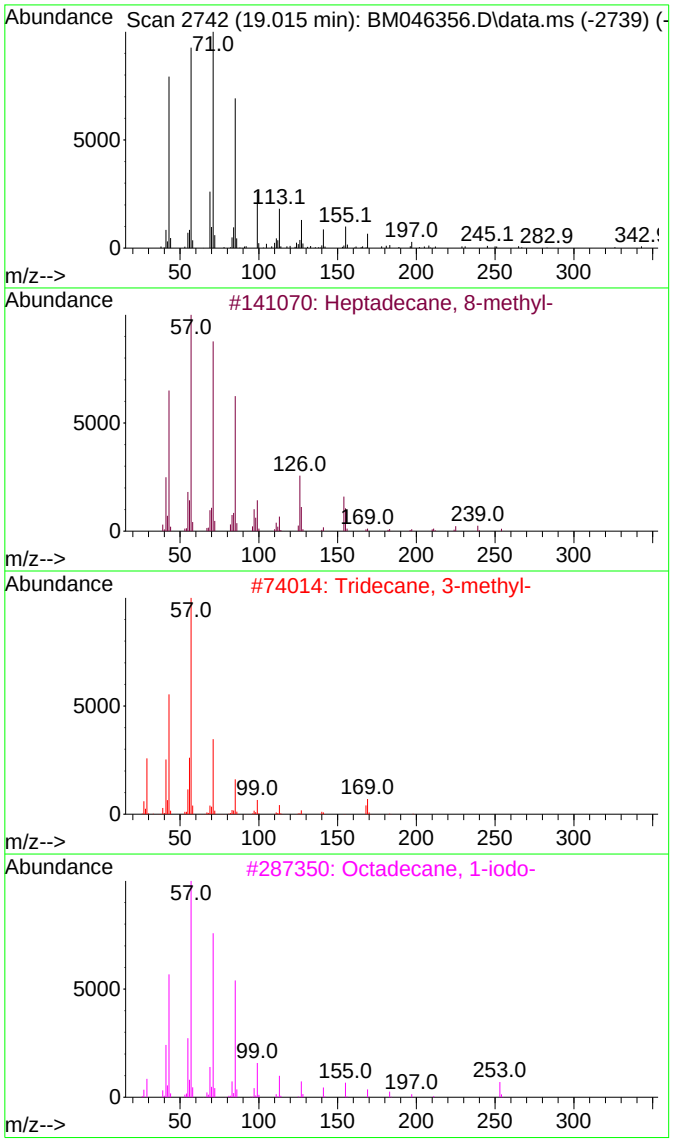
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

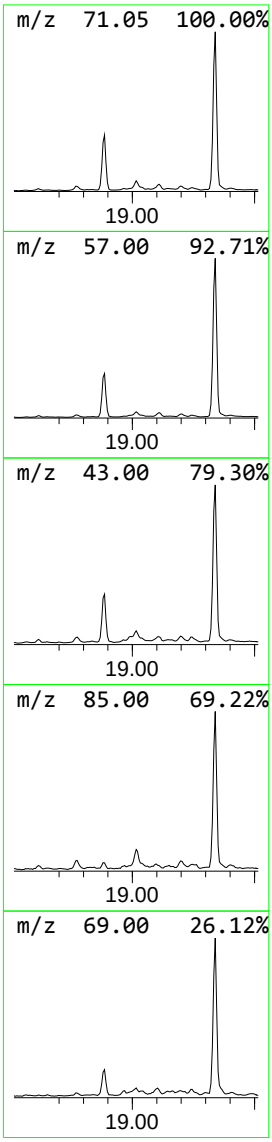
****

Peak Number 18 Heptadecane, 8-methyl- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.015	4.59 ng	290102	Chrysene-d12	20.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane, 8-methyl-	254	C18H38	013287-23-5	86
2	Tridecane, 3-methyl-	198	C14H30	006418-41-3	86
3	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	83
4	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	83
5	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	74





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046356.D
Acq On : 28 Jun 2024 17:23
Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

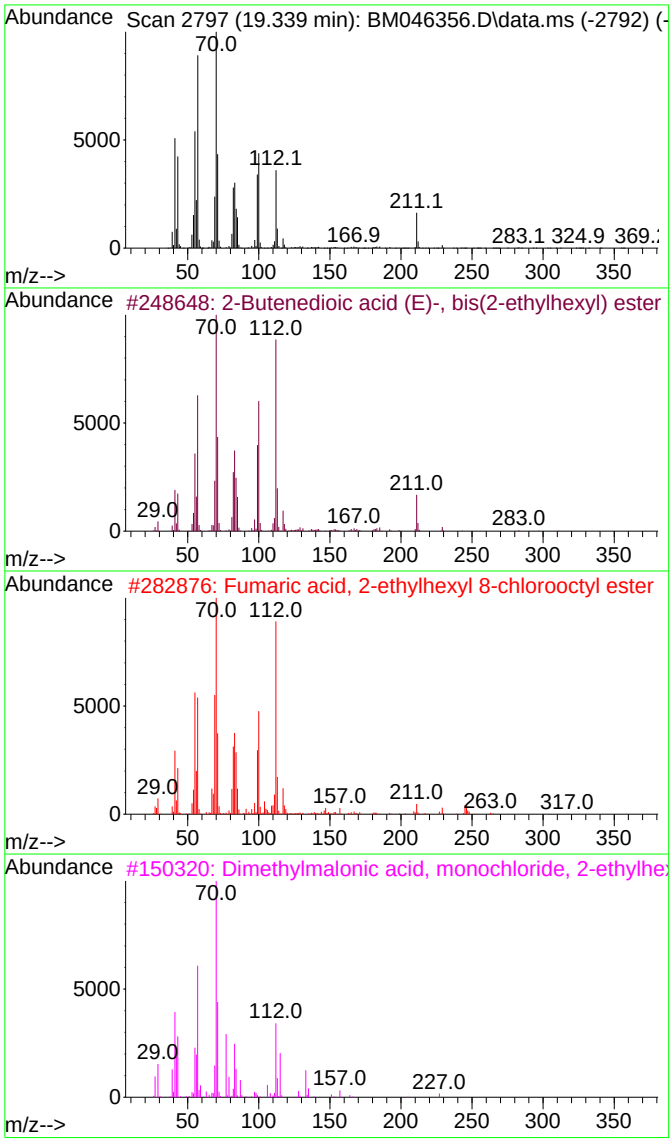
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

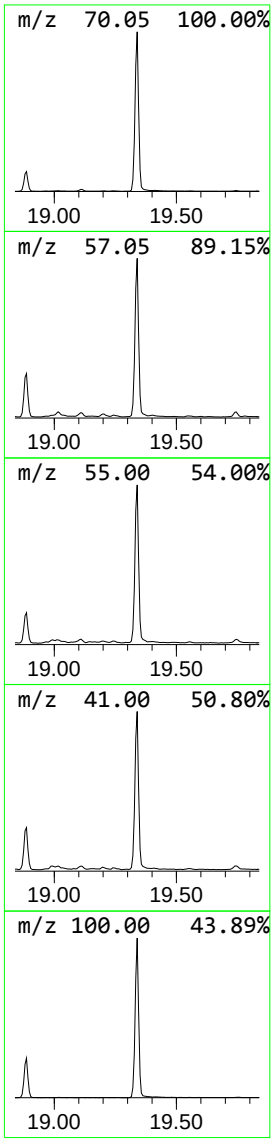
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 19 2-Butenedioic acid (E)-, bi... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.339	131.01 ng	8271780	Chrysene-d12	20.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenedioic acid (E)-, bis(2-e...	340	C20H36O4	000141-02-6	91
2	Fumaric acid, 2-ethylhexyl 8-chl...	374	C20H35ClO4	1000405-57-8	59
3	Dimethylmalonic acid, monochlori...	262	C13H23ClO3	1000361-64-8	47
4	Carbonic acid, butyl 2-ethylhexy...	230	C13H26O3	1000357-84-4	43
5	Cyclohexane, (1,1-dimethylpropyl)-	154	C11H22	031797-64-5	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046356.D
Acq On : 28 Jun 2024 17:23
Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

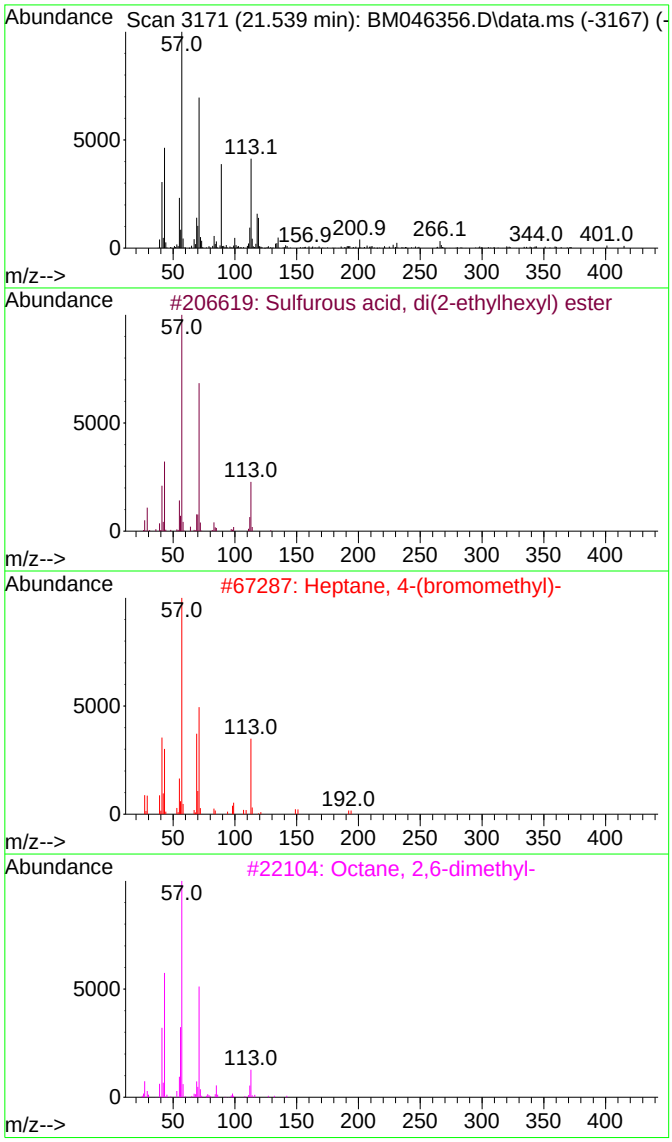
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

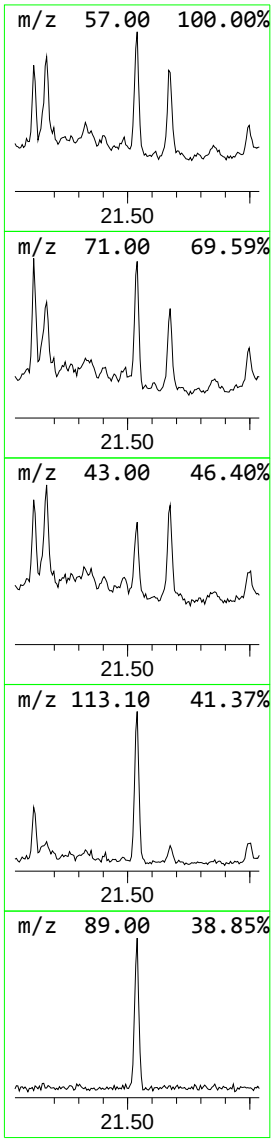
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 20 unknown21.539 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.539	4.53 ng	285769	Chrysene-d12	20.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sulfurous acid, di(2-ethylhexyl)...	306	C16H34O3S	1000309-19-1	43
2	Heptane, 4-(bromomethyl)-	192	C8H17Br	101654-29-9	43
3	Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	38
4	Sulfurous acid, 2-ethylhexyl iso...	250	C12H26O3S	1000309-18-7	38
5	5,11-Diethyl-8-methyl-7,9-dioxap...	286	C18H38O2	1000334-83-1	37





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM062824\
Data File : BM046356.D
Acq On : 28 Jun 2024 17:23
Operator : MA/JU
Sample : P3049-01 10X
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
SHOP-RAG-DRUM

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM062724.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown6.375	6.375	4.7	ng	280280	1	7.369	1203030	20.0
Benzene, 1-ethy...	6.475	5.0	ng	298369	1	7.369	1203030	20.0
Nonane	6.999	9.3	ng	562082	1	7.369	1203030	20.0
Benzene, 1,2,3-...	7.475	4.6	ng	277110	1	7.369	1203030	20.0
Benzene, (1-met...	7.904	5.0	ng	300368	1	7.369	1203030	20.0
Benzene, 1,4-di...	8.004	5.3	ng	321539	1	7.369	1203030	20.0
Hexanoic acid, ...	8.916	86.1	ng	7582140	2	10.128	1760880	20.0
Di-tert-butyl d...	9.098	7.3	ng	646719	2	10.128	1760880	20.0
1-Propanol, 2-(...	10.698	10.9	ng	959120	2	10.128	1760880	20.0
2-Propanol, 1-(...	10.763	12.7	ng	1116560	2	10.128	1760880	20.0
Trisulfide, bis...	11.763	44.8	ng	3943410	2	10.128	1760880	20.0
1H-Benzotriazol...	14.392	17.4	ng	1520930	3	14.016	1751130	20.0
1H-Benzotriazol...	14.822	22.7	ng	1986770	3	14.016	1751130	20.0
n-Hexadecanoic ...	17.704	8.5	ng	688740	4	16.774	1612500	20.0
Bis(2-ethylhexy...	18.886	31.1	ng	1962050	5	20.992	1262740	20.0
Heptadecane, 8-...	19.015	4.6	ng	290102	5	20.992	1262740	20.0
2-Butenedioic a...	19.339	131.0	ng	8271780	5	20.992	1262740	20.0
unknown21.539	21.539	4.5	ng	285769	5	20.992	1262740	20.0