LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032322\
Data File : BM034343.D
Acq On : 23 Mar 2022 17:44
Operator : CG/JU
Sample : N2070-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument : BNA_M
ClientSampleId : 285

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-BM031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM034343.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.596	56	61	74	rBV	1189810	1651593	21.45%	2.988%
2	5.496	373	384	396	rBV	2724868	4020875	52.22%	7.274%
3	7.096	648	656	669	rBV	2653830	4198419	54.53%	7.595%
4	7.937	791	799	807	rBV	640635	983331	12.77%	1.779%
5	9.095	989	996	1005	rBV	1603533	2648960	34.40%	4.792%
6	10.748	1268	1277	1283	rBV	820274	1371509	17.81%	2.481%
7	11.072	1326	1332	1348	rBV	81209	212614	2.76%	0.385%
8	13.201	1687	1694	1705	rBV	3819827	5638742	73.24%	10.200%
9	14.295	1875	1880	1885	rBV	66567	105580	1.37%	0.191%
10	14.413	1894	1900	1908	rVB2	38009	81417	1.06%	0.147%
11	14.577	1921	1928	1934	rBV	1201546	1749906	22.73%	3.165%
12	16.060	2173	2180	2188	rBV	3253405	4633700	60.18%	8.382%
13	17.313	2387	2393	2397	rBV	1378745	2000509	25.98%	3.619%
14	17.354	2397	2400	2406	rVB	447473	618290	8.03%	1.118%
15	17.448	2411	2416	2420	rVB	93692	142872	1.86%	0.258%
16	17.712	2455	2461	2466	rBV2	34261	78166	1.02%	0.141%
17	18.212	2538	2546	2559	rBV2	686879	1243617	16.15%	2.250%
18	18.389	2570	2576	2579	rBV2	106057	199194	2.59%	0.360%
19	18.424	2579	2582	2587	rVB	90339	120104	1.56%	0.217%
20	18.489	2589	2593	2597	rBV6	45841	88813	1.15%	0.161%
21	18.965	2671	2674	2681	rVB2	52834	86931	1.13%	0.157%
22	19.065	2687	2691	2697	rBV	2145654	2771824	36.00%	5.014%
23	19.242	2718	2721	2728	rBV3	48909	82784	1.08%	0.150%
24	19.371	2738	2743	2750	rVB	883793	1192769	15.49%	2.158%
25	19.483	2758	2762	2772	rBV3	317737	502165	6.52%	0.908%
26	19.618	2781	2785	2793	rVB7	124373	214371	2.78%	0.388%
27	19.701	2795	2799	2800	rVV	127466	157421	2.04%	0.285%
28	19.730	2800	2804	2812	rVB	881429	1283541	16.67%	2.322%
29	19.930	2833	2838	2849	rVB	5942263	7699487	100.00%	13.928%
30	20.048	2855	2858	2866	rVB3	118325	237898	3.09%	0.430%
31	20.218	2883	2887	2894	rVB3	159611	258757	3.36%	0.468%
32	20.383	2912	2915	2918	rBV2	73412	84374	1.10%	0.153%
33	20.530	2935	2940	2943	rBV2	190058	307610	4.00%	0.556%
34	21.195	3050	3053	3061	rVB3	897831	1141699	14.83%	2.065%
35	21.489	3096	3103	3107	rBV2	1841740	3125041	40.59%	5.653%
36	21.524	3107	3109	3116	rVB	499841	586181	7.61%	1.060%

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032322\
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Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
285

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-BM031522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	23.165	3383	3388	3393	rBV	436114	969966	12.60%	1.755%
38	23.794	3491	3495	3505	rVB2	347837	688616	8.94%	1.246%
39	23.900	3507	3513	3520	rVV2	1096391	2101039	27.29%	3.801%

Sum of corrected areas: 55280685

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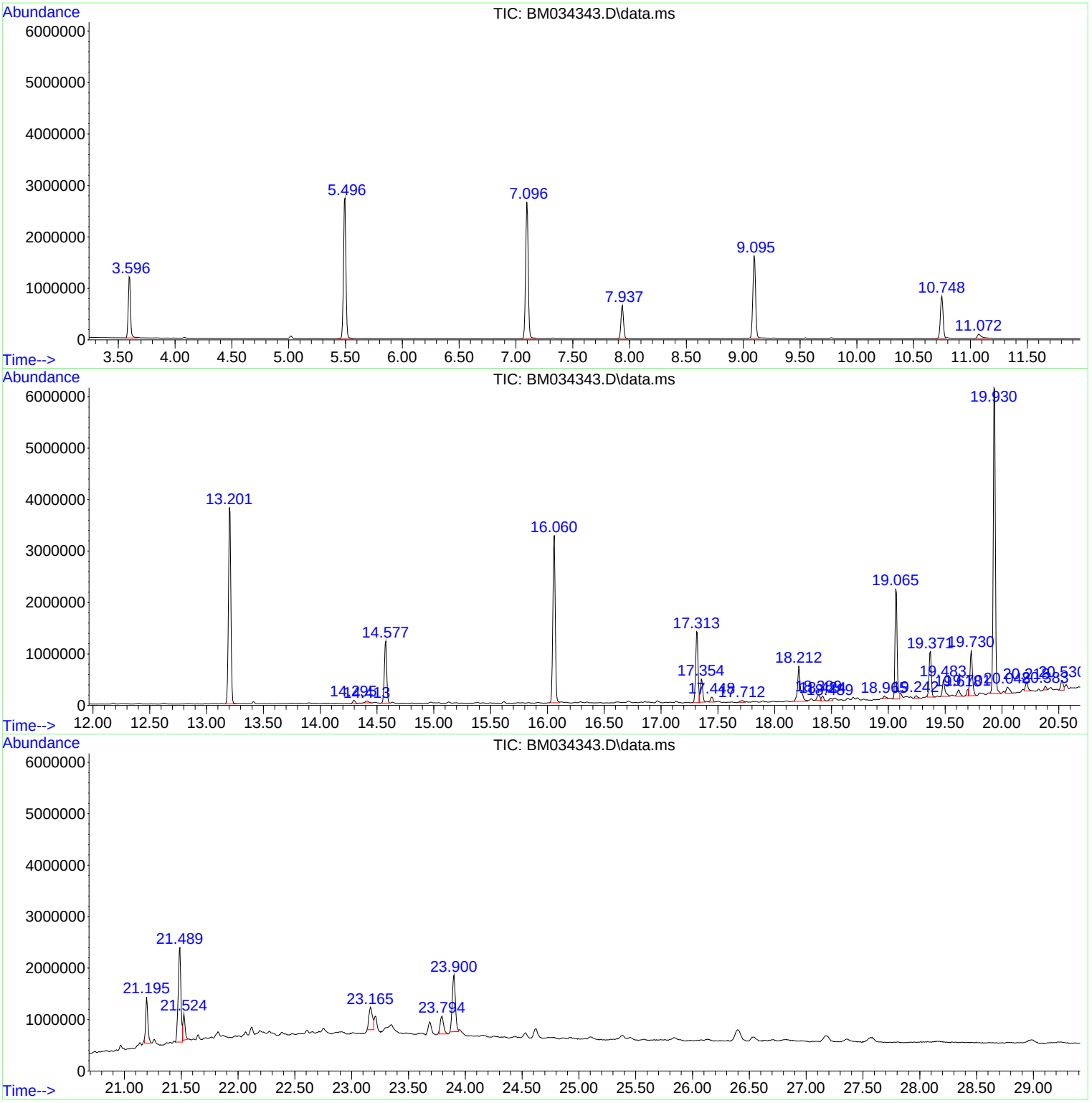
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BM034343.D
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

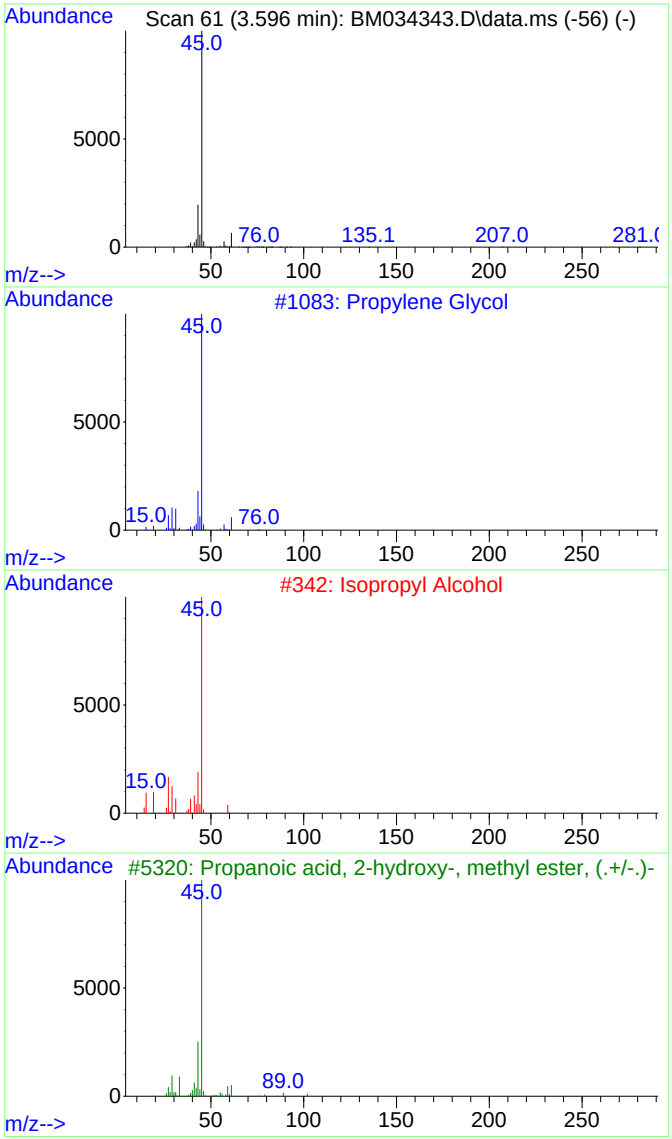
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

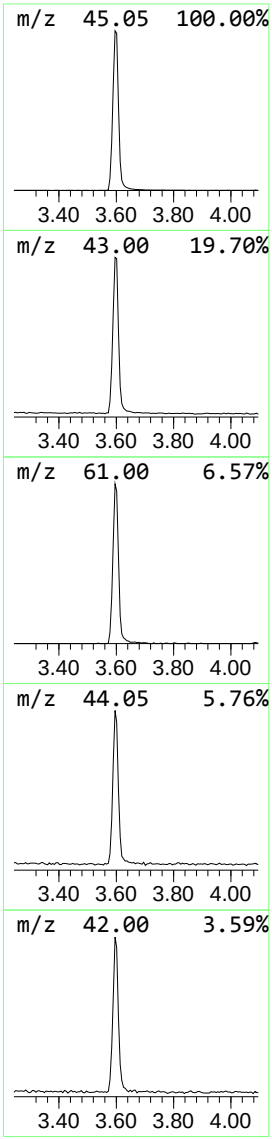
****

Peak Number 1 Propylene Glycol Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.596	33.59 ng	1651590	1,4-Dichlorobenzene-d4	7.937

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	90
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	56
3	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	40
4	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	40
5	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM032322\
Data File : BM034343.D
Acq On : 23 Mar 2022 17:44
Operator : CG/JU
Sample : N2070-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
285

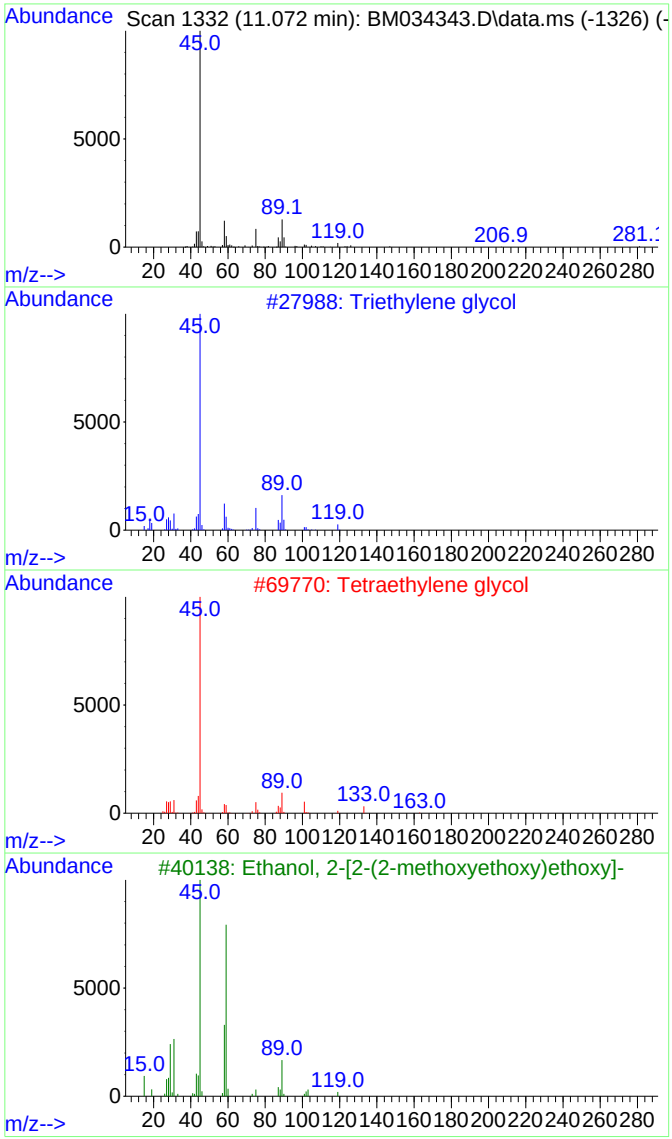
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

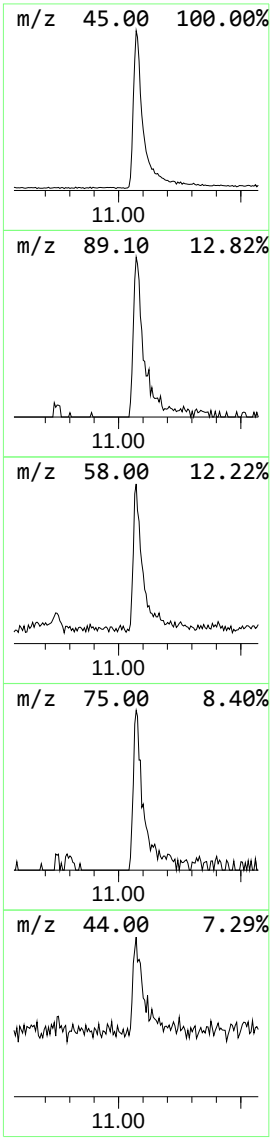
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 Triethylene glycol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.072	3.10 ng	212614	Naphthalene-d8	10.748

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triethylene glycol	150	C6H14O4	000112-27-6	90
2	Tetraethylene glycol	194	C8H18O5	000112-60-7	72
3	Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	64
4	Formic acid, 1-methylpropyl ester	102	C5H10O2	000589-40-2	53
5	Ethanol, 2-[2-(2-ethoxyethoxy)et...	178	C8H18O4	000112-50-5	45





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Sample : N2070-01
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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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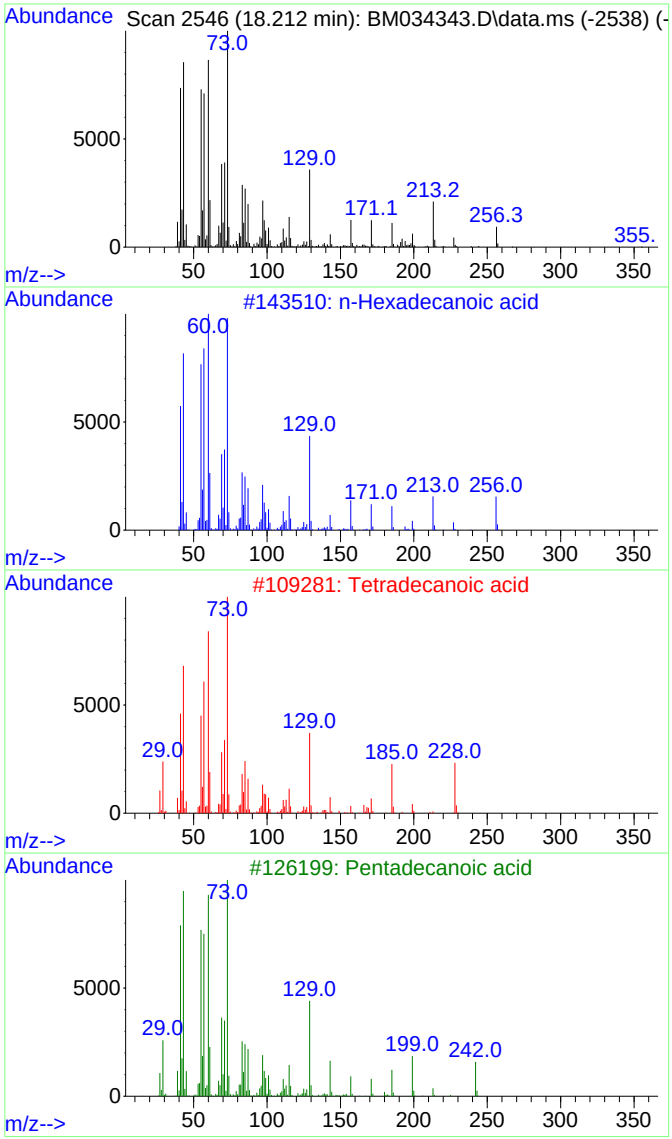
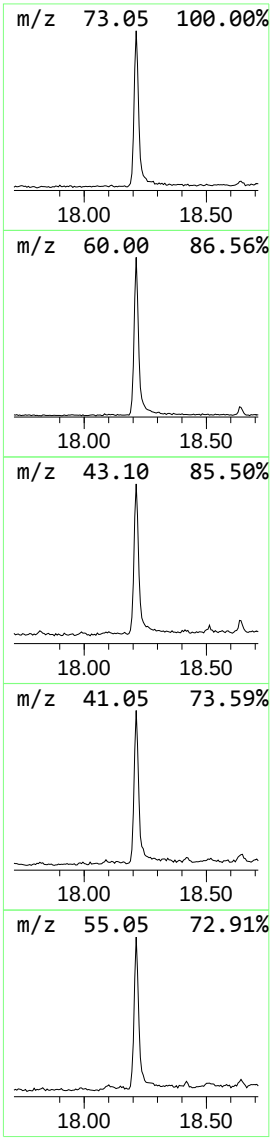
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.212	12.43 ng	1243620	Phenanthrene-d10	17.313

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	91
4	Tridecanoic acid	214	C13H26O2	000638-53-9	87
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	60





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
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TIC Library : C:\Database\NIST20.L
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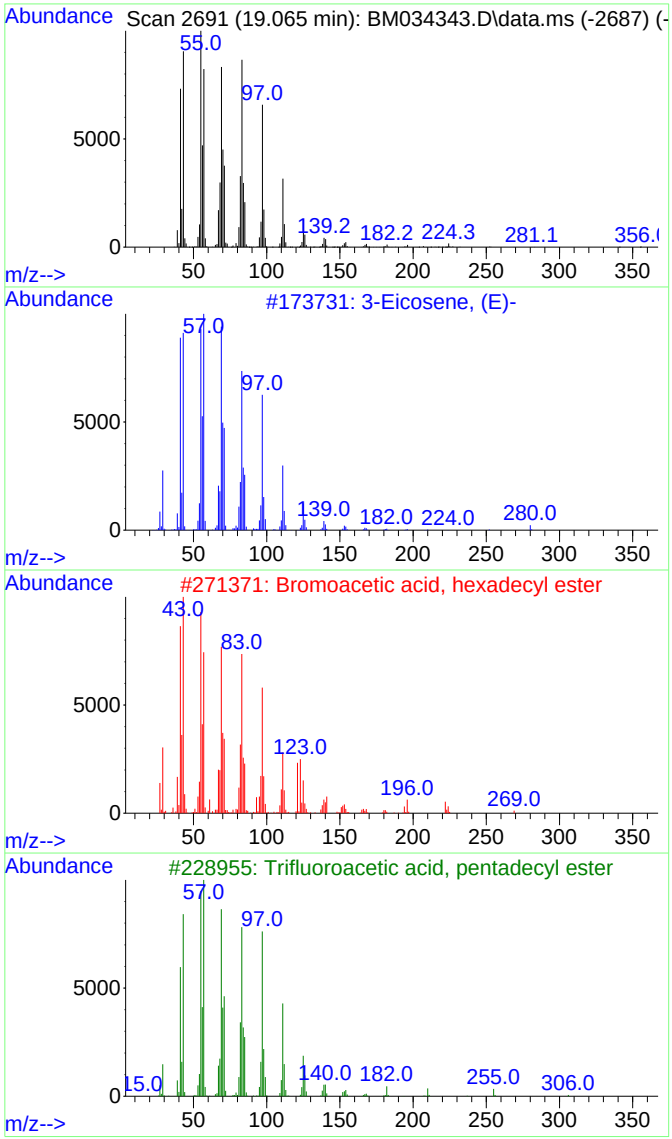
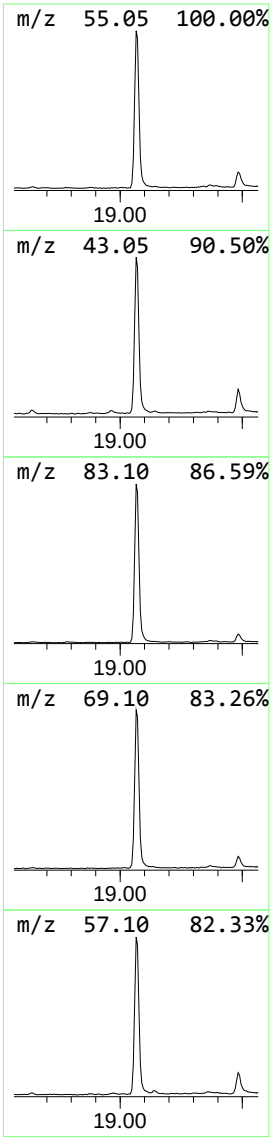
Peak Number 4 3-Eicosene, (E)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.065	27.71 ng	2771820	Phenanthrene-d10	17.313

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Eicosene, (E)-	280	C20H40	074685-33-9	95
2	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	94
3	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
4	9-Eicosene, (E)-	280	C20H40	074685-29-3	94
5	n-Nonadecanol-1	284	C19H40O	001454-84-8	94





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Sample : N2070-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
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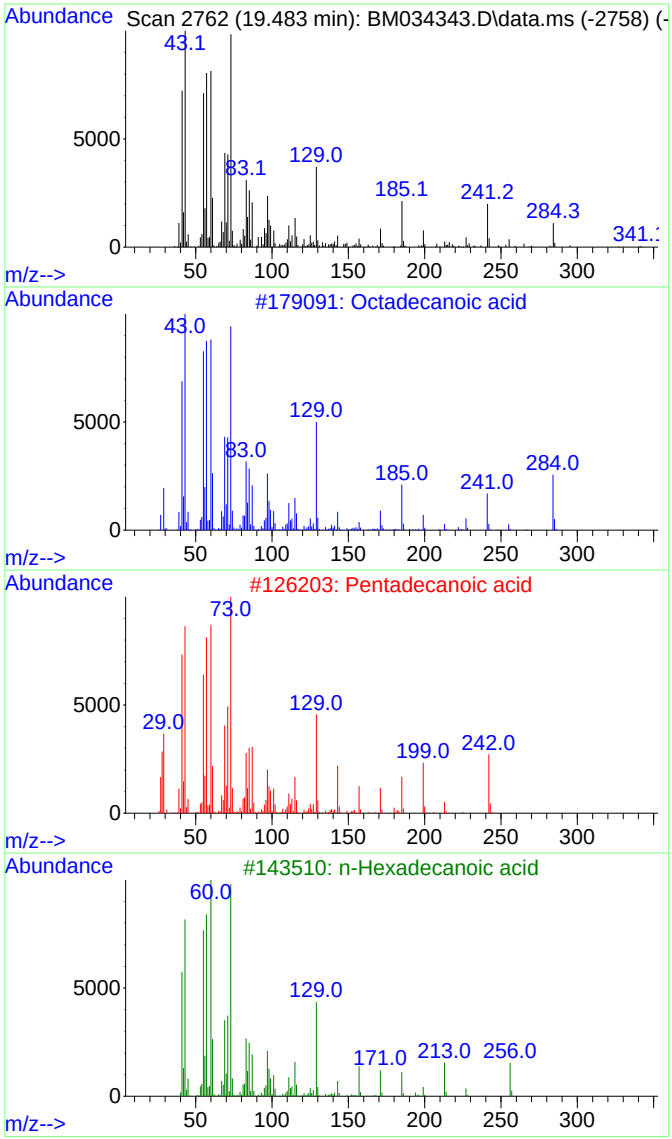
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM031522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

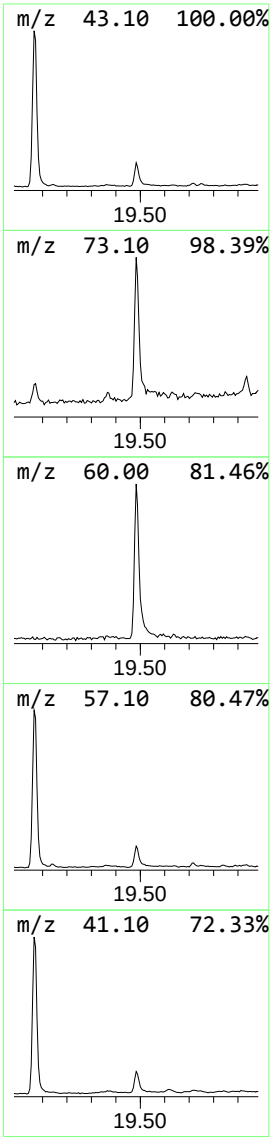
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.483	3.21 ng	502165	Chrysene-d12	21.489

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	81
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	80
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	74





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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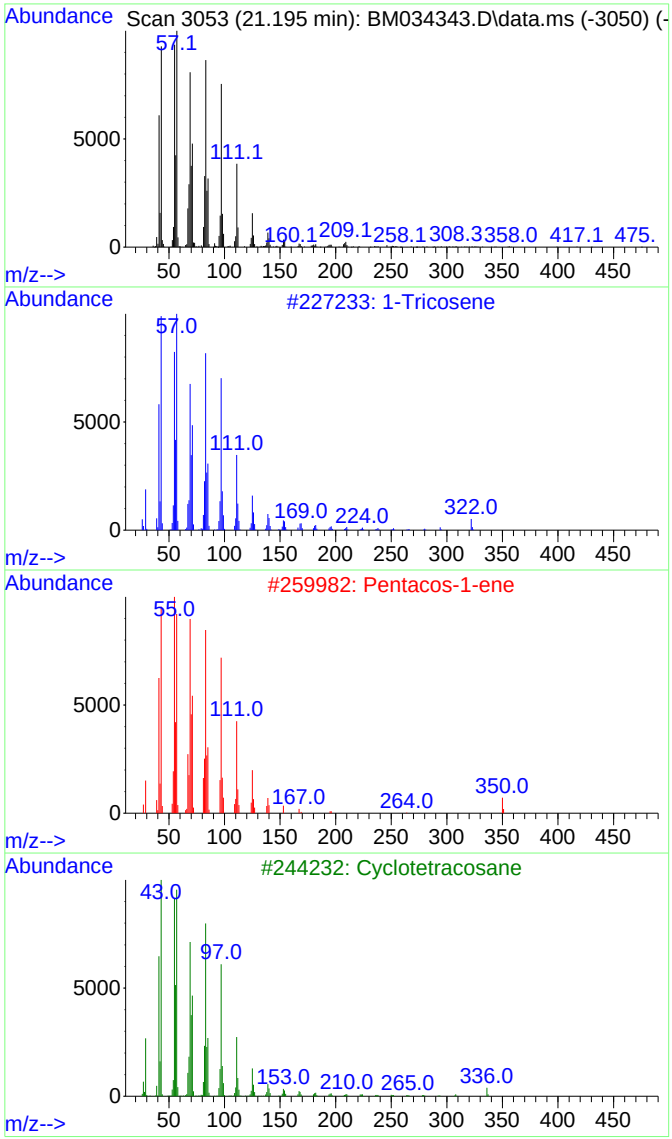
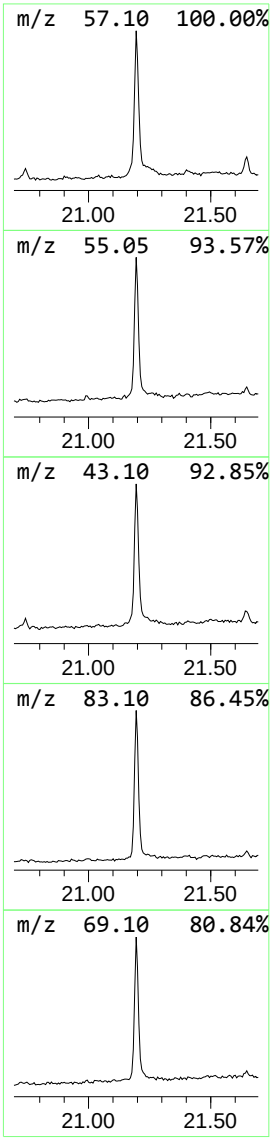
Peak Number 6 1-Tricosene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.195	7.31 ng	1141700	Chrysene-d12	21.489

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Tricosene	322	C23H46	018835-32-0	97
2	Pentacos-1-ene	350	C25H50	016980-85-1	94
3	Cyclotetracosane	336	C24H48	000297-03-0	93
4	n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5	1-Hexacosene	364	C26H52	018835-33-1	91





Tentatively Identified Compound (LSC) summary

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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
Propylene Glycol	3.596	33.6	ng	1651590	1	7.937	983331	20.0
Triethylene glycol	11.072	3.1	ng	212614	2	10.748	1371510	20.0
n-Hexadecanoic ...	18.212	12.4	ng	1243620	4	17.313	2000510	20.0
3-Eicosene, (E)-	19.065	27.7	ng	2771820	4	17.313	2000510	20.0
Octadecanoic acid	19.483	3.2	ng	502165	5	21.489	3125040	20.0
1-Tricosene	21.195	7.3	ng	1141700	5	21.489	3125040	20.0