LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_M\Data\BM082924\
Data File : BM047394.D
Acq On : 29 Aug 2024 15:06
Operator : RC/JU
Sample : P3775-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-865-N-SO-1-1.5-082824

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-BM082624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BM047394.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.257	60	63	75	rVB	58354	91312	1.29%	0.148%
2	4.557	276	284	290	rBV	130413	188986	2.67%	0.307%
3	5.004	354	360	380	rBV	1974693	2926125	41.34%	4.748%
4	6.569	619	626	641	rBV	1875933	3115824	44.02%	5.056%
5	7.345	747	758	770	rBV	824689	1338808	18.91%	2.172%
6	8.492	945	953	963	rBV	1293518	2133588	30.14%	3.462%
7	10.098	1217	1226	1236	rBV	1040210	1747648	24.69%	2.836%
8	10.869	1349	1357	1367	rBV	107406	236841	3.35%	0.384%
9	12.610	1646	1653	1665	rBV	3239923	4888078	69.05%	7.932%
10	14.004	1884	1890	1898	rBV	1657824	2517733	35.57%	4.085%
11	14.239	1925	1930	1932	rBV4	61568	94766	1.34%	0.154%
12	14.480	1966	1971	1979	rBV2	143862	231161	3.27%	0.375%
13	14.863	2029	2036	2048	rVB	316939	556993	7.87%	0.904%
14	15.057	2064	2069	2075	rVB5	34685	73392	1.04%	0.119%
15	15.410	2123	2129	2137	rVB	112162	196015	2.77%	0.318%
16	15.521	2142	2148	2157	rBV	2894729	4346479	61.40%	7.053%
17	15.927	2213	2217	2224	rBV3	52292	102677	1.45%	0.167%
18	16.215	2262	2266	2273	rBV	151872	236179	3.34%	0.383%
19	16.562	2321	2325	2328	rBV2	67598	88044	1.24%	0.143%
20	16.727	2349	2353	2356	rBV	107109	139755	1.97%	0.227%
21	16.774	2356	2361	2365	rVV	2231361	3054573	43.15%	4.957%
22	16.815	2365	2368	2374	rVB	256281	335875	4.74%	0.545%
23	16.904	2379	2383	2389	rVB2	122522	207255	2.93%	0.336%
24	16.986	2393	2397	2402	rBV2	90471	133584	1.89%	0.217%
25	17.086	2410	2414	2420	rVB	114158	158241	2.24%	0.257%
26	17.192	2430	2432	2447	rVB2	70643	151938	2.15%	0.247%
27	17.580	2494	2498	2503	rBV7	60434	115928	1.64%	0.188%
28	17.715	2513	2521	2527	rBV	4301112	6988394	98.72%	11.340%
29	17.768	2527	2530	2539	rVB	521201	863694	12.20%	1.401%
30	18.133	2587	2592	2595	rBV3	97546	140050	1.98%	0.227%
31	18.256	2609	2613	2622	rVB	176949	265659	3.75%	0.431%
32	18.580	2665	2668	2675	rVB4	81335	120936	1.71%	0.196%
33	18.851	2710	2714	2729	rBV	874075	1454995	20.55%	2.361%
34	19.009	2736	2741	2753	rBV	2367517	3724246	52.61%	6.043%
35	19.221	2769	2777	2782	rVV	770763	1325277	18.72%	2.150%
36	19.274	2782	2786	2797	rVB2	179791	350528	4.95%	0.569%

LSC Area Percent Report

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Data File : BM047394.D
Acq On : 29 Aug 2024 15:06
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Sample : P3775-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-865-N-SO-1-1.5-082824

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-BM082624.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	19.439	2809	2814	2819	rBV	5568553	7078975	100.00%	11.487%
38	19.727	2860	2863	2869	rVB2	129847	192781	2.72%	0.313%
39	19.833	2878	2881	2886	rBV2	98284	133282	1.88%	0.216%
40	20.745	3033	3036	3041	rVB	548084	653366	9.23%	1.060%
41	20.950	3067	3071	3075	rBV	550288	675138	9.54%	1.096%
42	21.015	3076	3082	3087	rVV2	2448895	3915105	55.31%	6.353%
43	21.056	3087	3089	3098	rVB	445464	561397	7.93%	0.911%
44	22.874	3393	3398	3404	rBV	282928	693293	9.79%	1.125%
45	23.715	3534	3541	3559	rVB	1252937	3082632	43.55%	5.002%

Sum of corrected areas: 61627546

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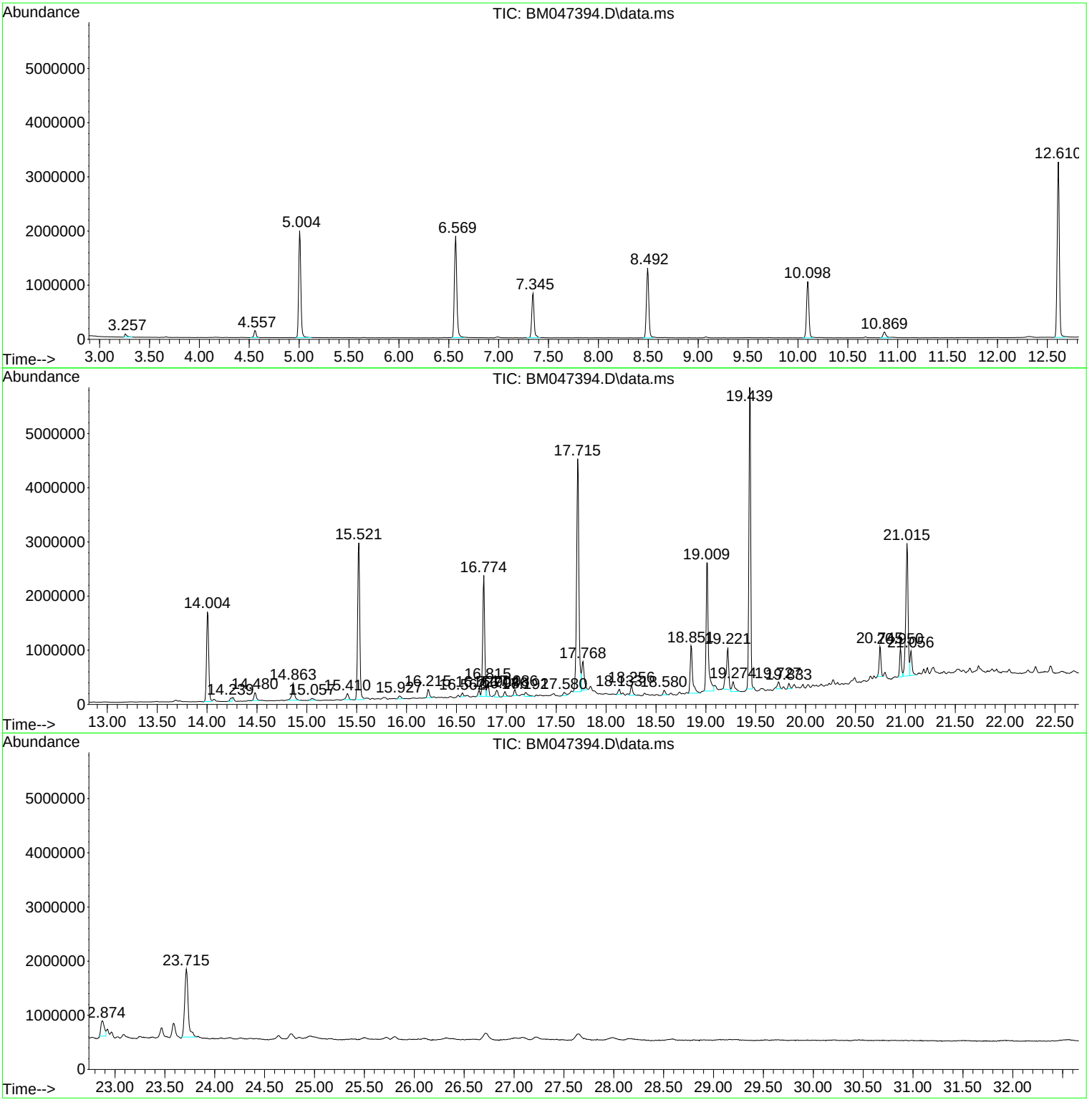
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-865-N-SO-1-1.5-082824

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.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\BM082924\
Data File : BM047394.D
Acq On : 29 Aug 2024 15:06
Operator : RC/JU
Sample : P3775-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_M
ClientSampleId :
S-865-N-SO-1-1.5-082824

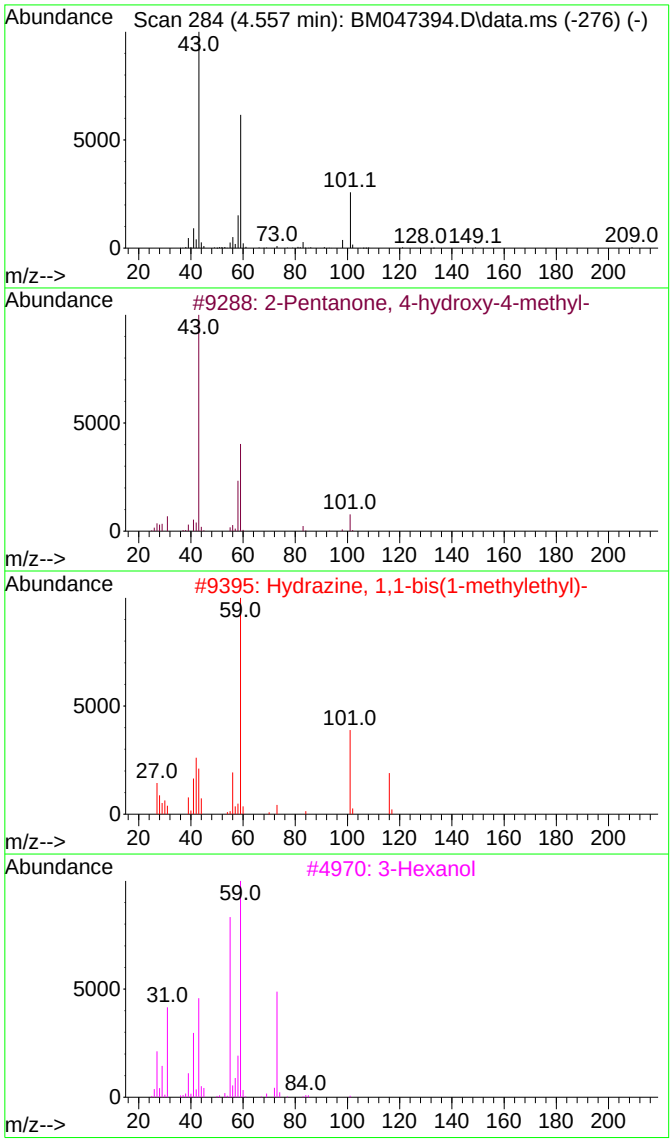
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

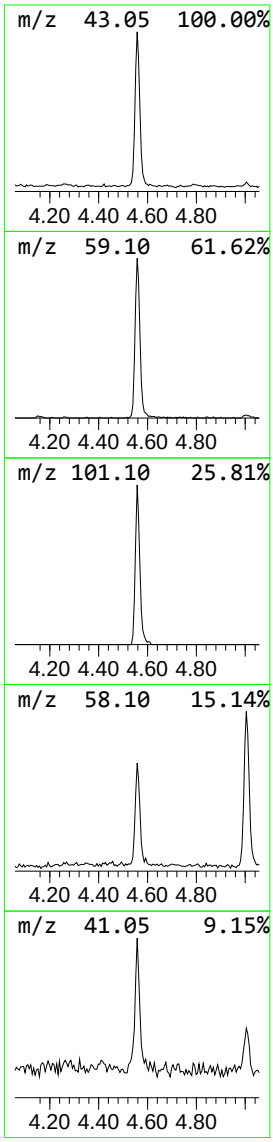
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.557	2.82 ng	188986	1,4-Dichlorobenzene-d4	7.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	28
3	3-Hexanol	102	C6H14O	000623-37-0	28
4	1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
5	Tetraglyme	222	C10H22O5	000143-24-8	23





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S-865-N-SO-1-1.5-082824

Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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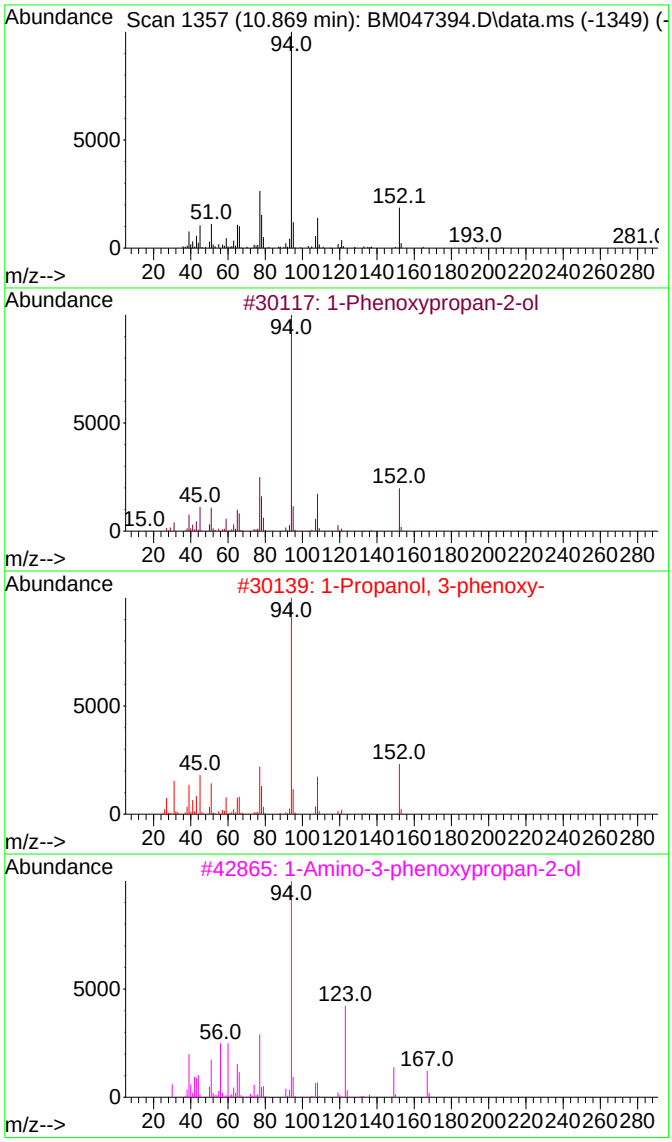
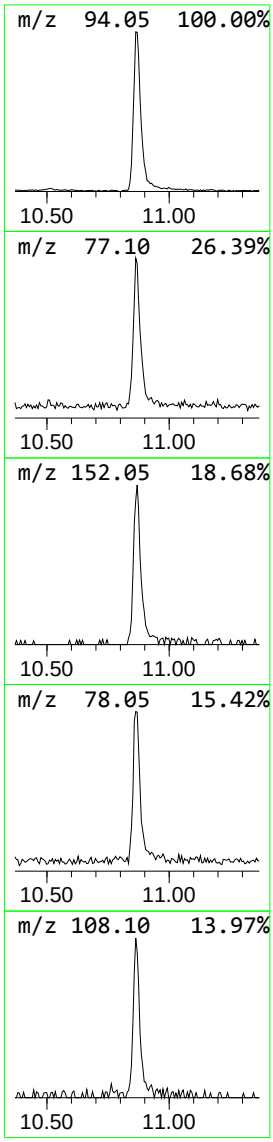
****

Peak Number 2 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.869	2.71 ng	236841	Naphthalene-d8	10.098

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	94
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3	1-Amino-3-phenoxypropan-2-ol	167	C9H13NO2	004287-19-8	64
4	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	64
5	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

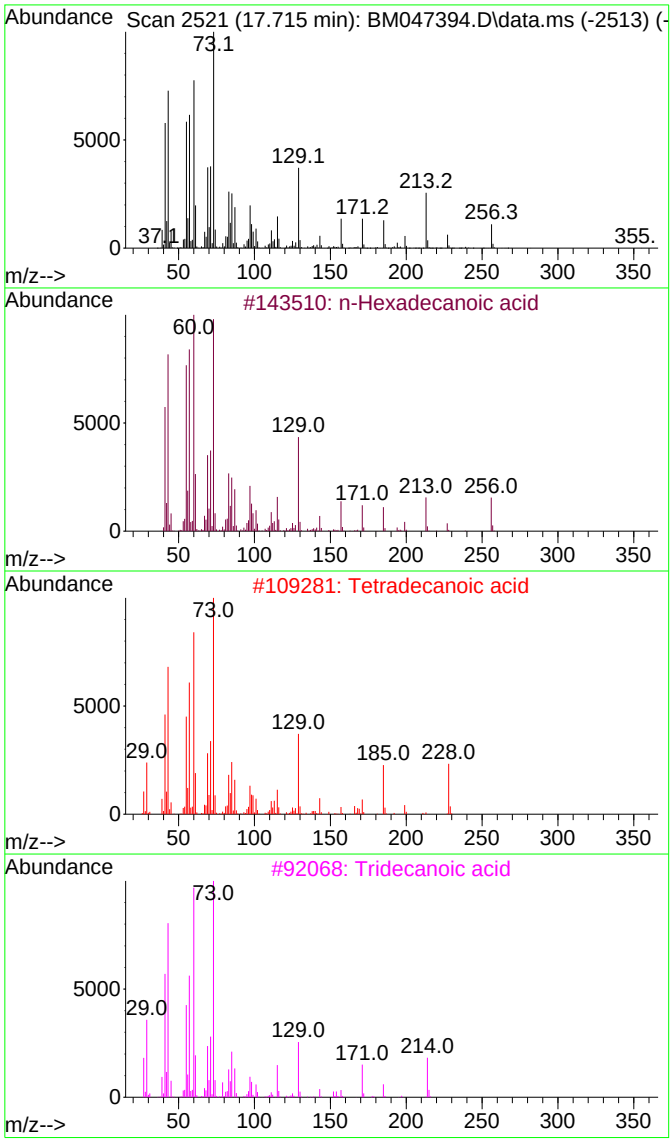
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

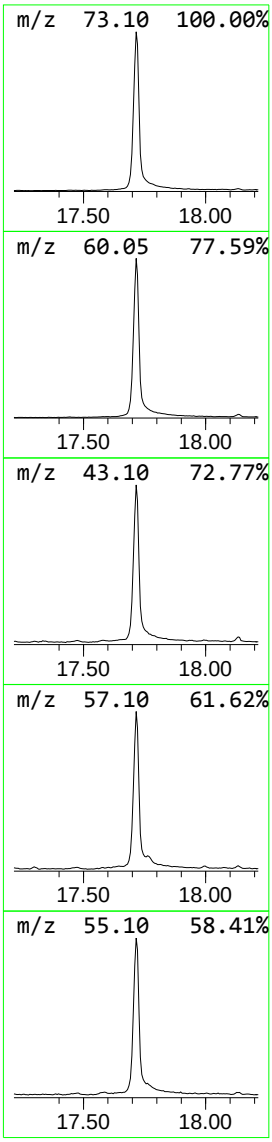
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.715	45.76 ng	6988390	Phenanthrene-d10	16.774

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	93
3	Tridecanoic acid	214	C13H26O2	000638-53-9	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
5	n-Decanoic acid	172	C10H20O2	000334-48-5	64





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Instrument :
BNA_M
ClientSampleId :
S-865-N-SO-1-1.5-082824

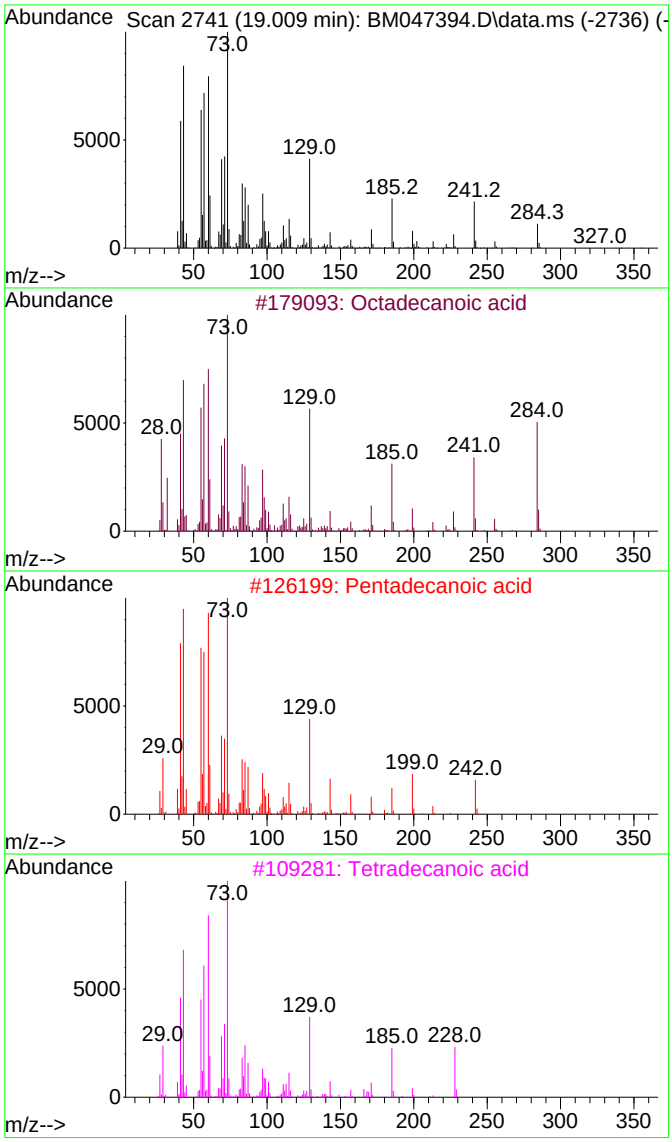
Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

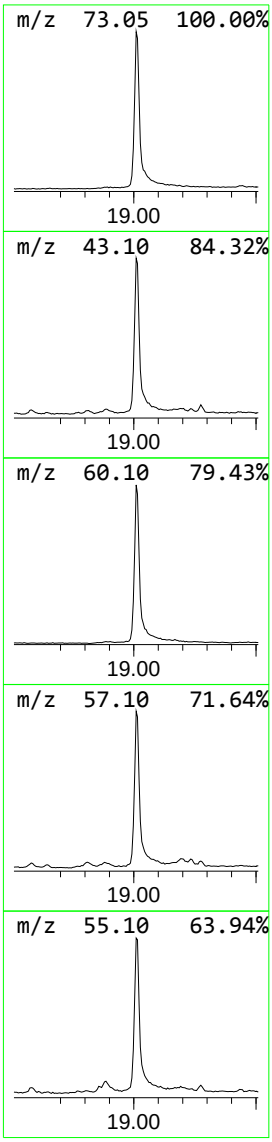
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.009	19.02 ng	3724250	Chrysene-d12	21.015

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	Tetradecanoic acid	228	C14H28O2	000544-63-8	87
4	n-Decanoic acid	172	C10H20O2	000334-48-5	62
5	Tridecane	184	C13H28	000629-50-5	25





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_M\Methods\8270-BM082624.M
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TIC Library : C:\Database\NIST20.L
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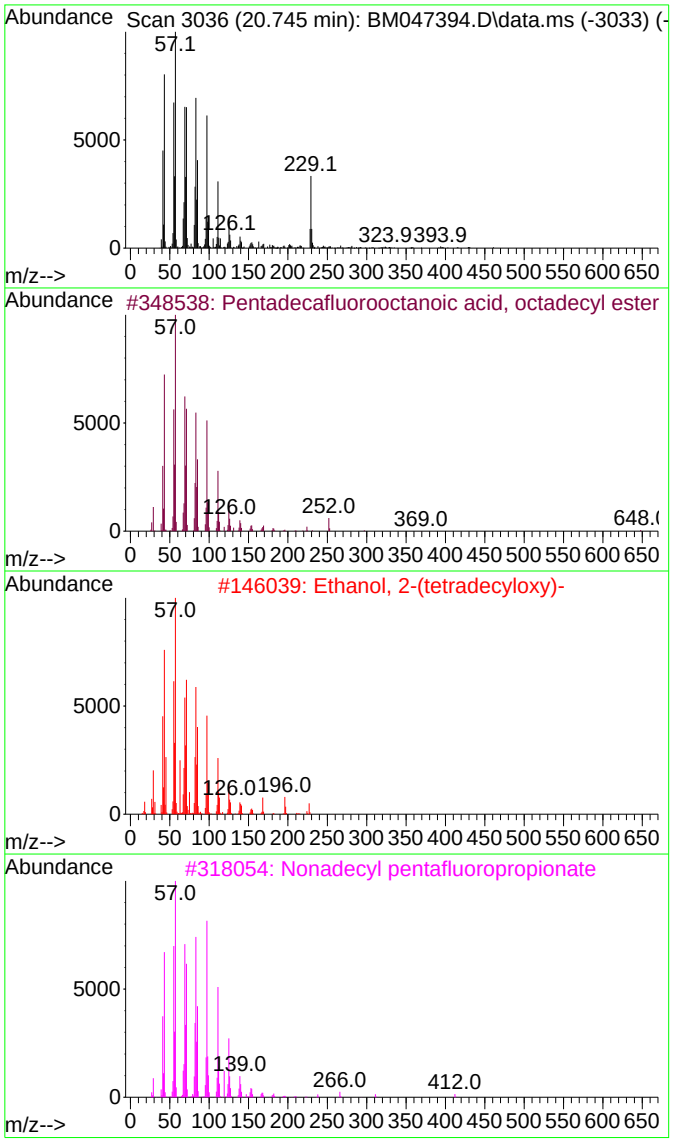
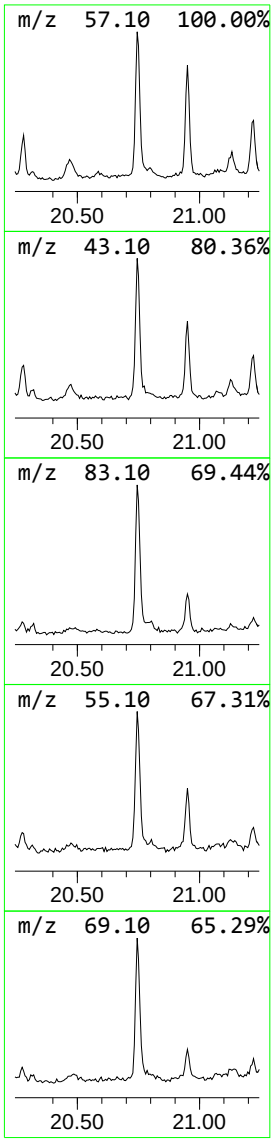
****
Peak Number 5 Pentadecafluorooctanoic aci... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.744	3.34 ng	653366	Chrysene-d12	21.015

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecafluorooctanoic acid, oc...	666	C26H37F15O2	1000406-04-8	91
2	Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
3	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	87
4	Nonadecyl trifluoroacetate	380	C21H39F3O2	1000351-76-3	87
5	9-Eicosene, (E)-	280	C20H40	074685-29-3	83





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
2-Pentanone, 4-...	4.557	2.8	ng	188986	1	7.345	1338810	20.0
1-Phenoxypropan...	10.869	2.7	ng	236841	2	10.098	1747650	20.0
n-Hexadecanoic ...	17.715	45.8	ng	6988390	4	16.774	3054570	20.0
Octadecanoic acid	19.009	19.0	ng	3724250	5	21.015	3915110	20.0
Pentadecafluoro...	20.744	3.3	ng	653366	5	21.015	3915110	20.0