LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051925\
Data File : BF142447.D
Acq On : 19 May 2025 13:08
Operator : RC/JU
Sample : Q2032-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-29

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_F\Methods\8270-BF050525.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF142447.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.428	205	210	229	rBV	35009	92699	2.79%	0.422%
2	5.116	488	497	505	rVB	173970	262310	7.89%	1.194%
3	5.516	559	565	570	rBV	1571774	2067053	62.20%	9.407%
4	6.522	729	736	741	rBV	1565290	2151527	64.75%	9.792%
5	6.728	766	771	781	rBV	27674	39277	1.18%	0.179%
6	6.898	795	800	806	rBV	639206	813456	24.48%	3.702%
7	7.457	889	895	901	rBV	989114	1327575	39.95%	6.042%
8	8.181	1013	1018	1034	rBV	826612	1089019	32.77%	4.956%
9	8.492	1066	1071	1081	rBV	99389	138896	4.18%	0.632%
10	9.257	1195	1201	1206	rBV	1946870	2420254	72.83%	11.015%
11	9.939	1311	1317	1322	rBV	997364	1232441	37.09%	5.609%
12	10.033	1326	1333	1339	rBV	2026504	3322973	100.00%	15.123%
13	10.651	1432	1438	1444	rBV	95240	119524	3.60%	0.544%
14	10.727	1445	1451	1463	rBV	1306003	1687714	50.79%	7.681%
15	11.427	1564	1570	1577	rBV	924193	1233736	37.13%	5.615%
16	11.945	1651	1658	1671	rBV2	121377	205879	6.20%	0.937%
17	12.639	1772	1776	1779	rBV	34714	41320	1.24%	0.188%
18	12.733	1784	1792	1800	rBV2	24909	41530	1.25%	0.189%
19	12.868	1810	1815	1818	rBV	27574	39822	1.20%	0.181%
20	13.010	1833	1839	1844	rBV	1605914	2043985	61.51%	9.302%
21	13.904	1986	1991	2007	rBV	46881	92637	2.79%	0.422%
22	14.063	2013	2018	2029	rVB	522216	725271	21.83%	3.301%
23	15.557	2266	2272	2289	rBV	493804	783612	23.58%	3.566%

Sum of corrected areas: 21972510

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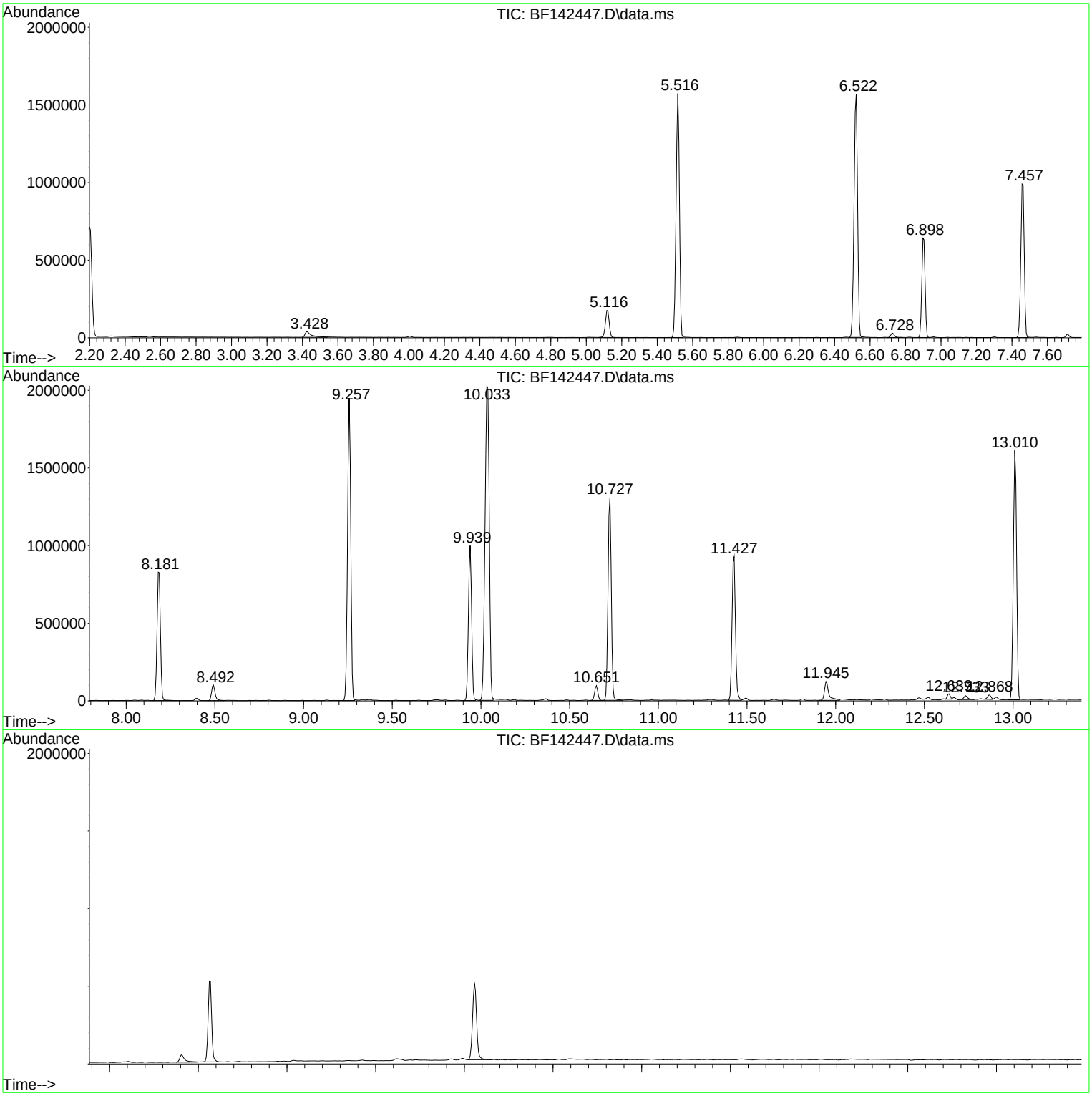
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Data File : BF142447.D
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TIC Library : C:\Database\NIST20.L
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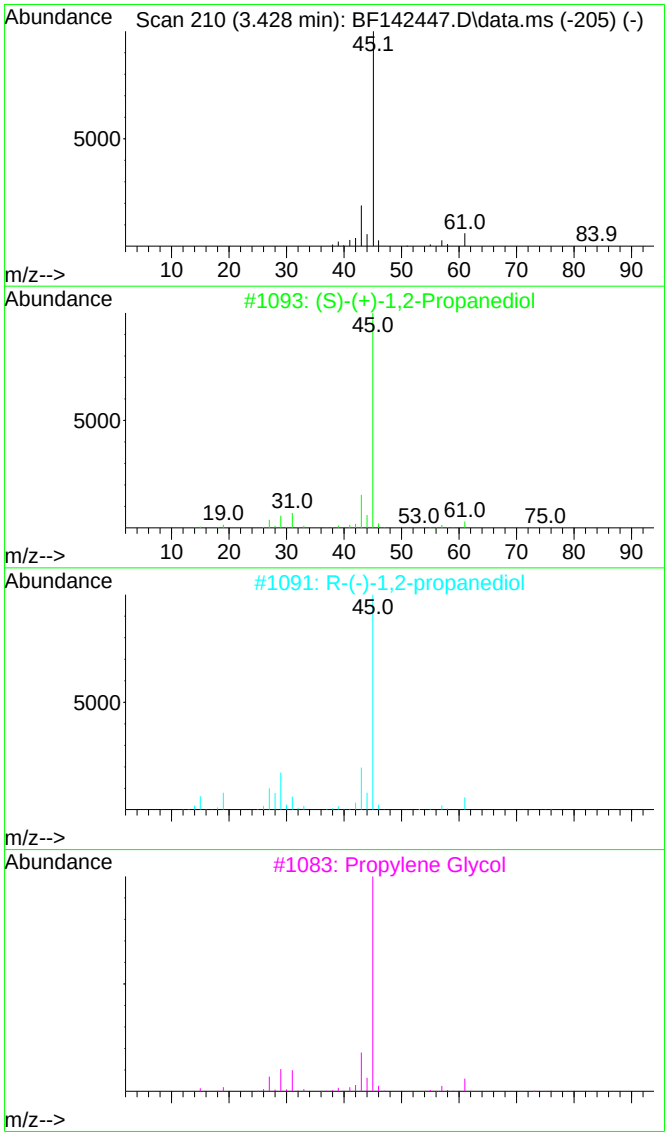
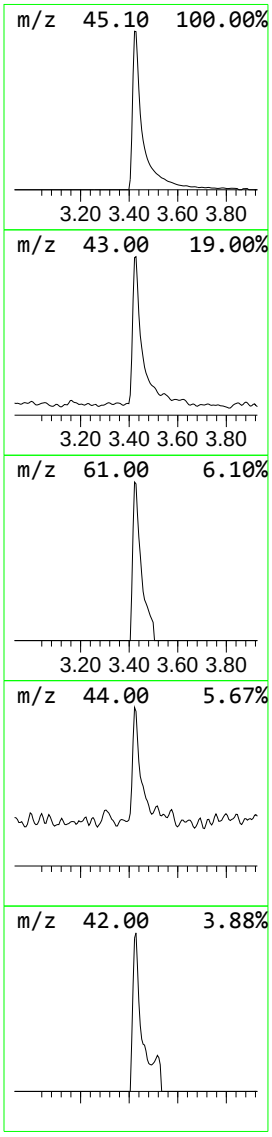
****

Peak Number 1 (S)-(+)-1,2-Propanediol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.428	2.28 ng	92699	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
2	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
3	Propylene Glycol	76	C3H8O2	000057-55-6	9
4	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
5	Formamide	45	CH3NO	000075-12-7	7





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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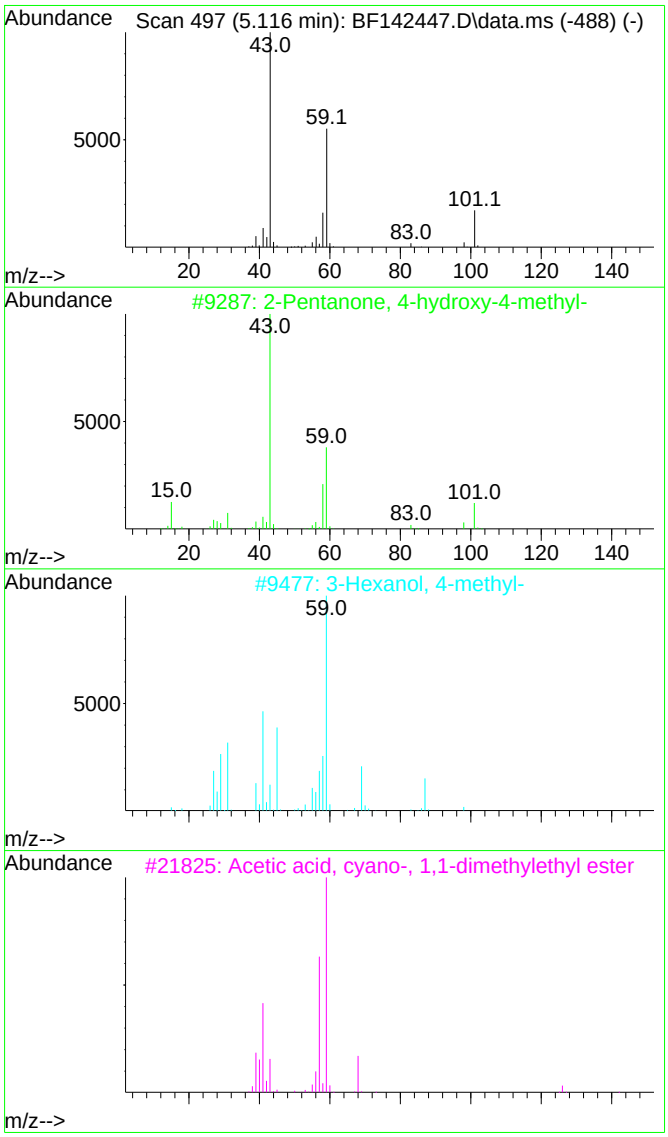
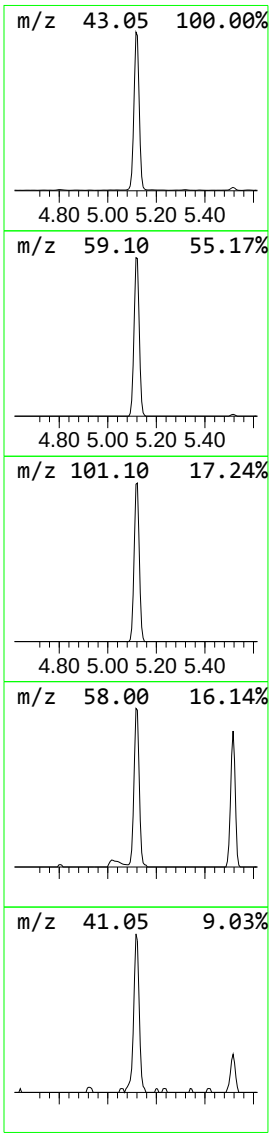
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	6.45 ng	262310	1,4-Dichlorobenzene-d4	6.904

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9





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Sample : Q2032-02
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF050525.M
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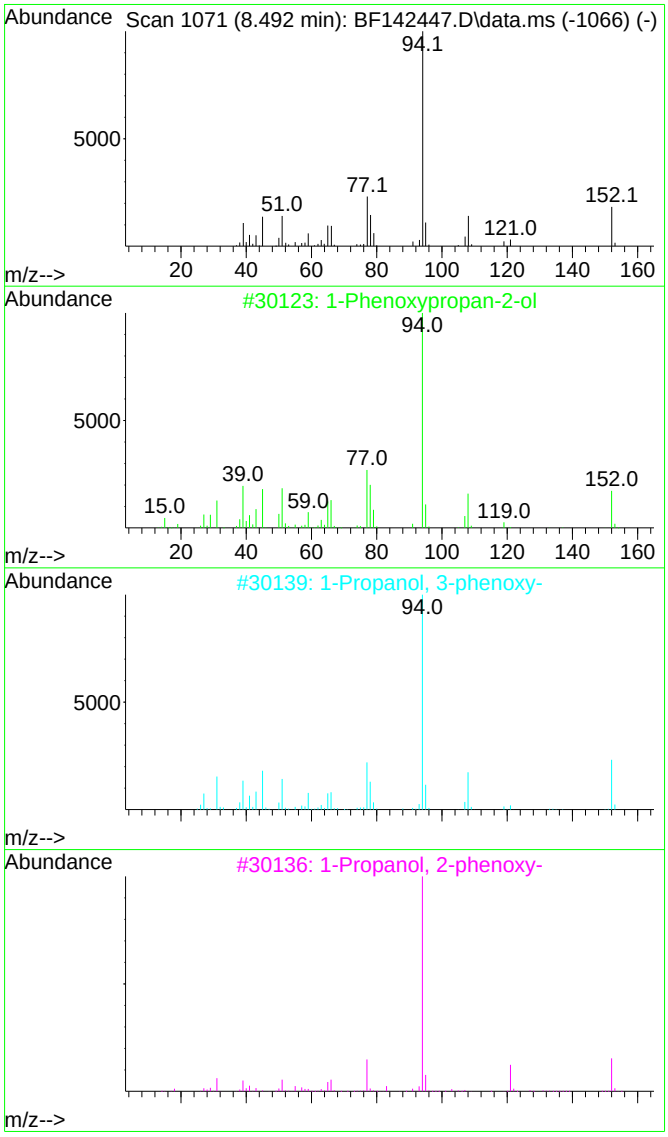
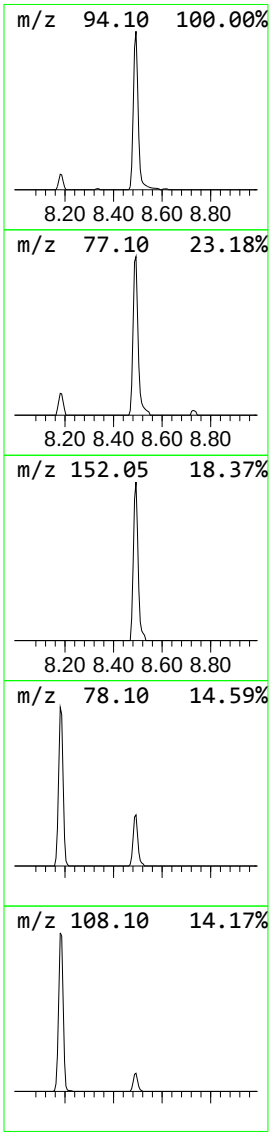
Peak Number 3 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.492	2.55 ng	138896	Naphthalene-d8	8.186

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	91
3	1-Propanol, 2-phenoxy-	152	C9H12O2	004169-04-4	64
4	Ethanol, 2-phenoxy-	138	C8H10O2	000122-99-6	64
5	Carbonic acid, neopentyl phenyl ...	208	C12H16O3	013183-19-2	59





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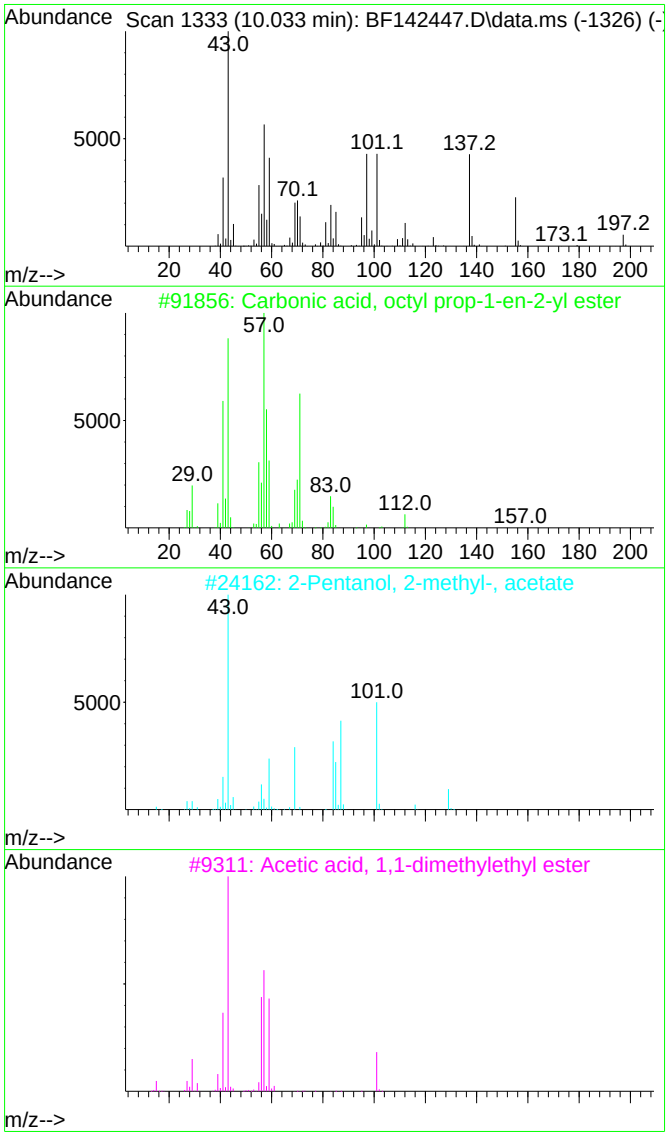
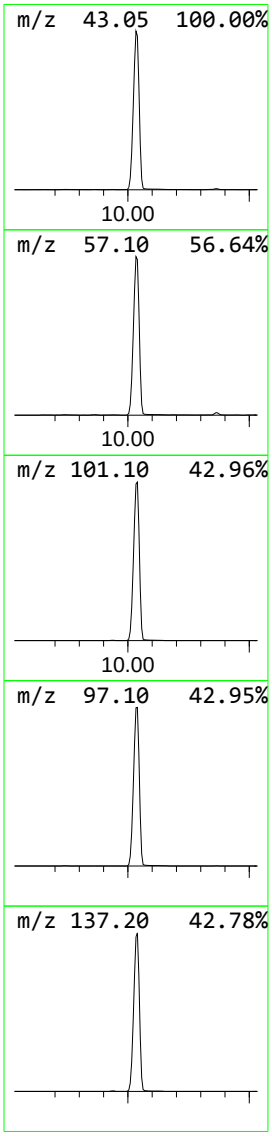
Peak Number 4 unknown10.033 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.033	53.93 ng	3322970	Acenaphthene-d10	9.939

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Carbonic acid, octyl prop-1-en-2...	214	C12H22O3	1000382-54-0	12
2	2-Pentanol, 2-methyl-, acetate	144	C8H16O2	034859-98-8	10
3	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	10
4	6,10,14-Trimethyl-pentadecan-2-ol	270	C18H38O	069729-17-5	10
5	11-Tricosene	322	C23H46	052078-56-5	10





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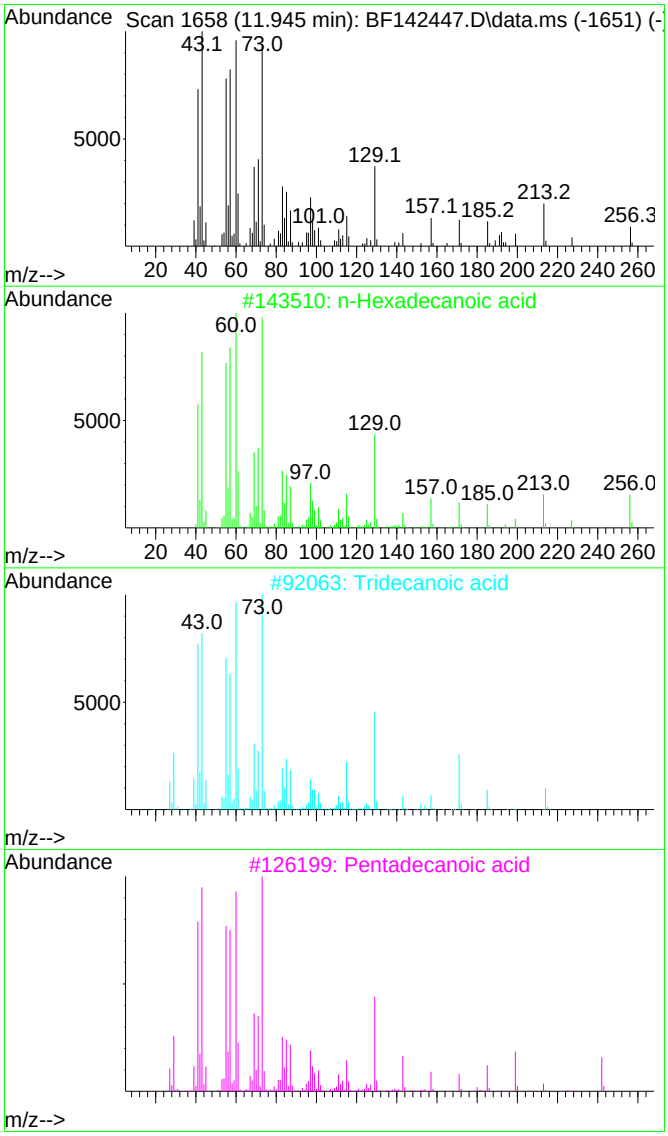
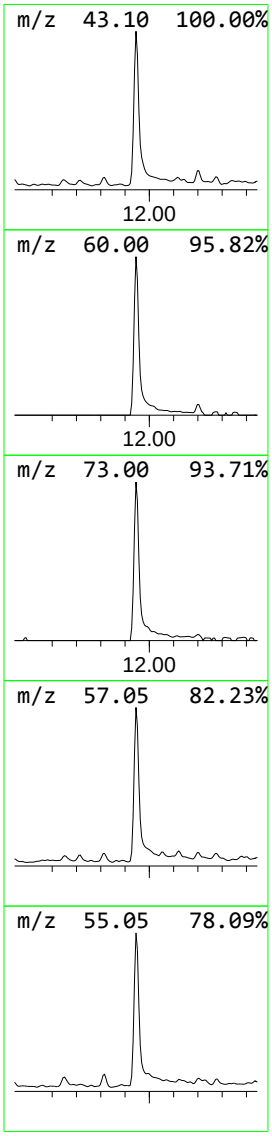
Peak Number 5 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	3.34 ng	205879	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	89
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	76
4	n-Decanoic acid	172	C10H20O2	000334-48-5	64
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	64





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TIC Library : C:\Database\NIST20.L
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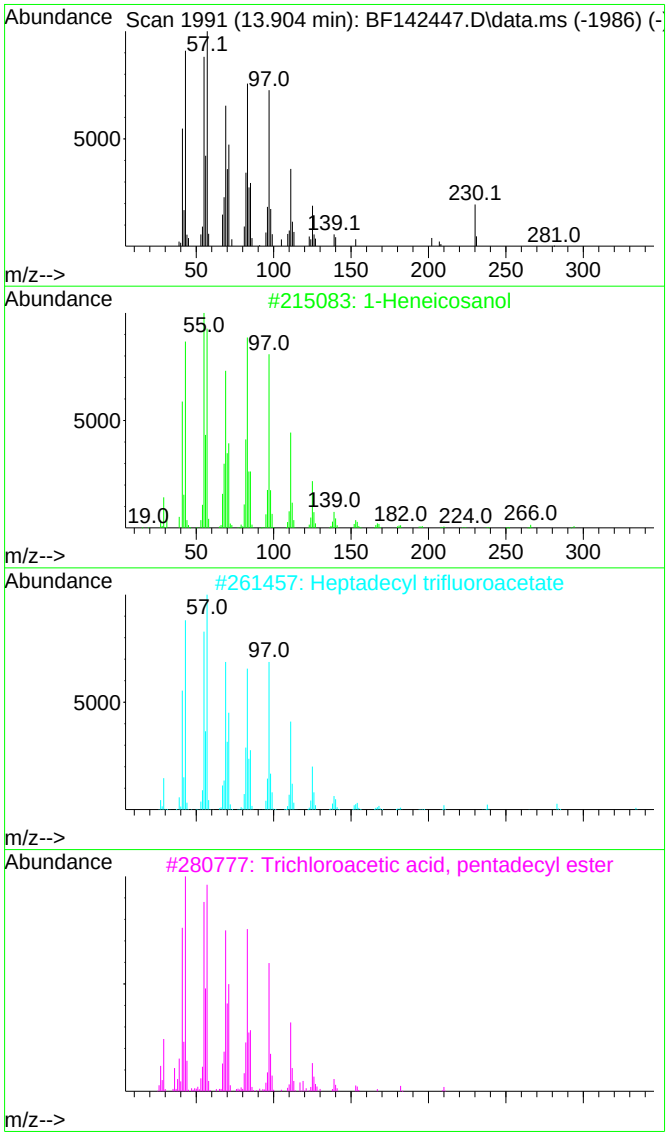
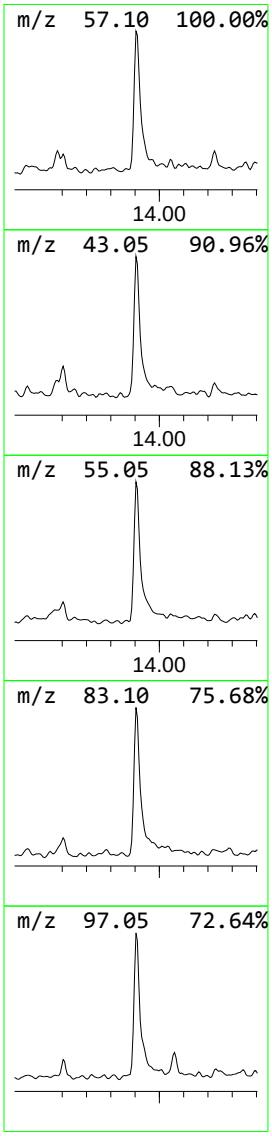
Peak Number 6 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	2.55 ng	92637	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	93
3	Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	90
4	1-Nonadecene	266	C19H38	018435-45-5	90
5	1-Hexacosene	364	C26H52	018835-33-1	90





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
(S)-(+)-1,2-Pro...	3.428	2.3	ng	92699	1	6.904	813456	20.0
2-Pentanone, 4-...	5.116	6.5	ng	262310	1	6.904	813456	20.0
1-Phenoxypropan...	8.492	2.5	ng	138896	2	8.186	1089020	20.0
unknown10.033	10.033	53.9	ng	3322970	3	9.939	1232440	20.0
n-Hexadecanoic ...	11.945	3.3	ng	205879	4	11.427	1233740	20.0
1-Heneicosanol	13.904	2.5	ng	92637	5	14.068	725271	20.0