LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF100523\
Data File : BF135612.D
Acq On : 05 Oct 2023 21:50
Operator : CG\JU
Sample : 04714-07
Misc :
ALS Vial : 16 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : TP-3

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-BF091123.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135612.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.963	484	489	506	rBV	892259	1242676	44.17%	6.173%
2	5.375	555	559	581	rBV	2755595	2813328	100.00%	13.975%
3	5.757	621	624	632	rVB	30673	31592	1.12%	0.157%
4	6.387	728	731	750	rBV	2734397	2778660	98.77%	13.803%
5	6.587	763	765	778	rVB	35112	60546	2.15%	0.301%
6	6.739	787	791	800	rBV	976346	855011	30.39%	4.247%
7	7.304	883	887	890	rBV	1993867	1686861	59.96%	8.379%
8	8.016	1005	1008	1022	rVB	1258695	1041403	37.02%	5.173%
9	9.092	1187	1191	1195	rBV	2851175	2373775	84.38%	11.792%
10	9.210	1208	1211	1216	rBV	55570	56310	2.00%	0.280%
11	9.769	1303	1306	1315	rBV	1071090	969648	34.47%	4.817%
12	10.569	1438	1442	1453	rBV	1220031	1232860	43.82%	6.124%
13	11.263	1557	1560	1564	rBV	915281	777049	27.62%	3.860%
14	11.798	1648	1651	1662	rBV2	182057	257936	9.17%	1.281%
15	12.592	1783	1786	1799	rBV2	31830	60176	2.14%	0.299%
16	12.857	1827	1831	1835	rBV	1644908	1436332	51.05%	7.135%
17	13.768	1982	1986	1988	rBV	40696	43369	1.54%	0.215%
18	13.810	1988	1993	2006	rVB2	68837	225485	8.01%	1.120%
19	13.921	2009	2012	2016	rBV	755824	720539	25.61%	3.579%
20	14.086	2036	2040	2043	rBV	28161	29962	1.07%	0.149%
21	14.392	2089	2092	2096	rVB	58742	54606	1.94%	0.271%
22	14.451	2096	2102	2117	rBV5	73385	248722	8.84%	1.236%
23	14.692	2140	2143	2147	rVB	32729	35778	1.27%	0.178%
24	15.027	2196	2200	2204	rVB	142849	161215	5.73%	0.801%
25	15.392	2257	2262	2274	rBV	576993	778451	27.67%	3.867%
26	15.839	2333	2338	2348	rVB	98730	158675	5.64%	0.788%

Sum of corrected areas: 20130965

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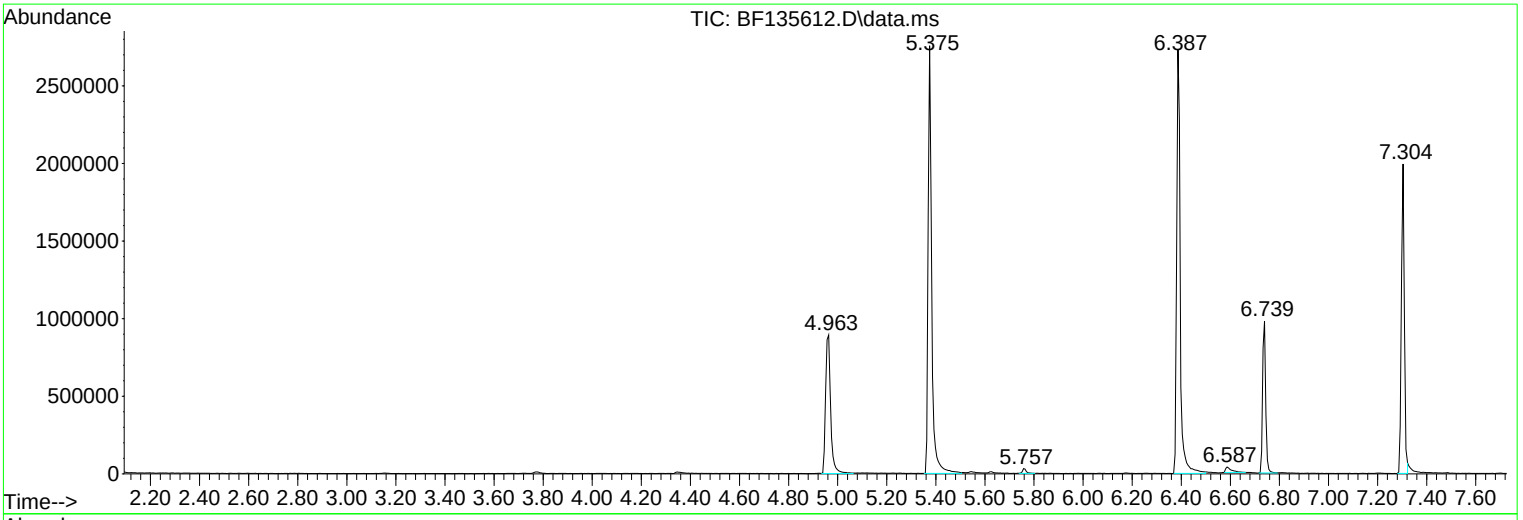
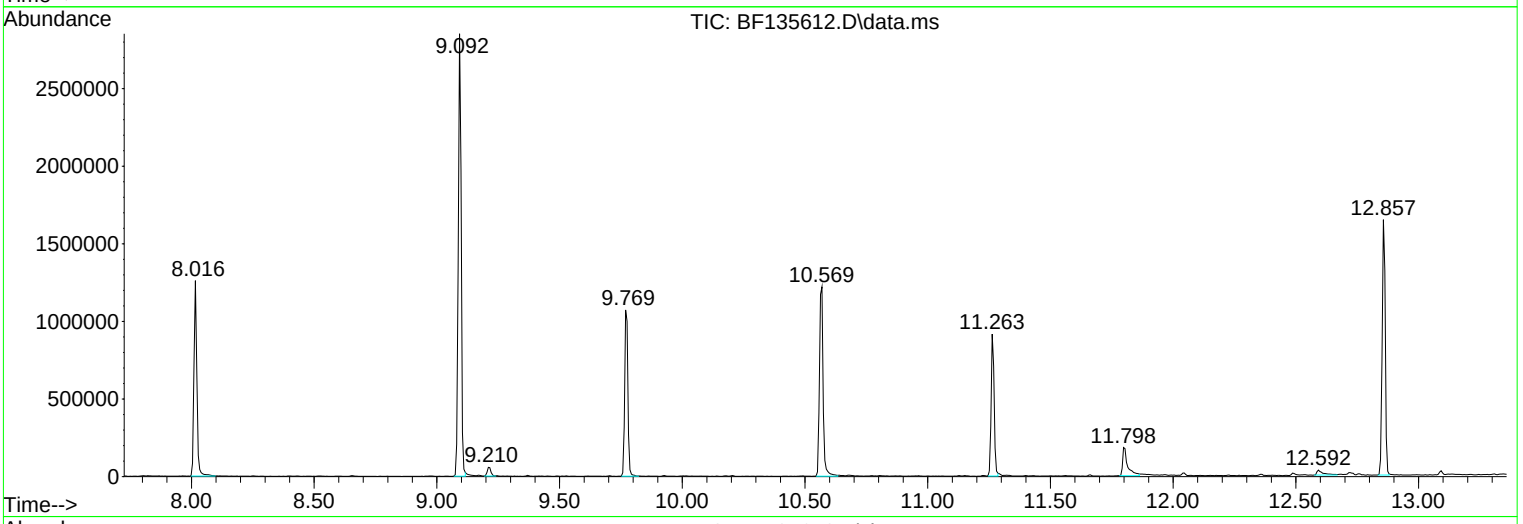
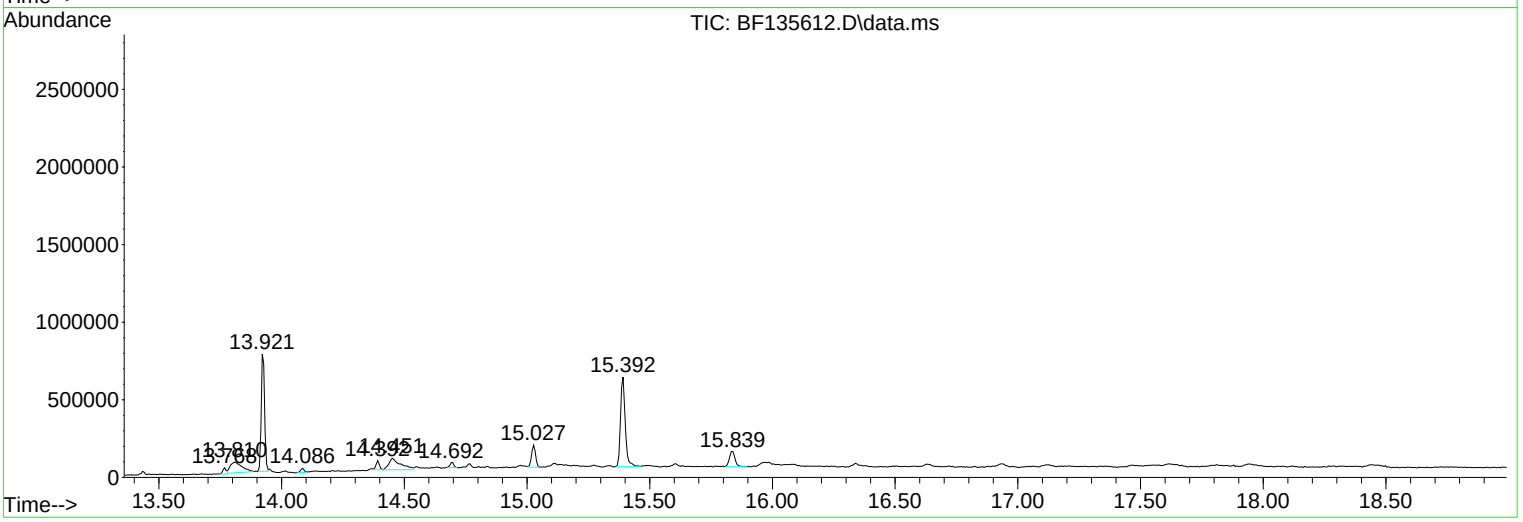
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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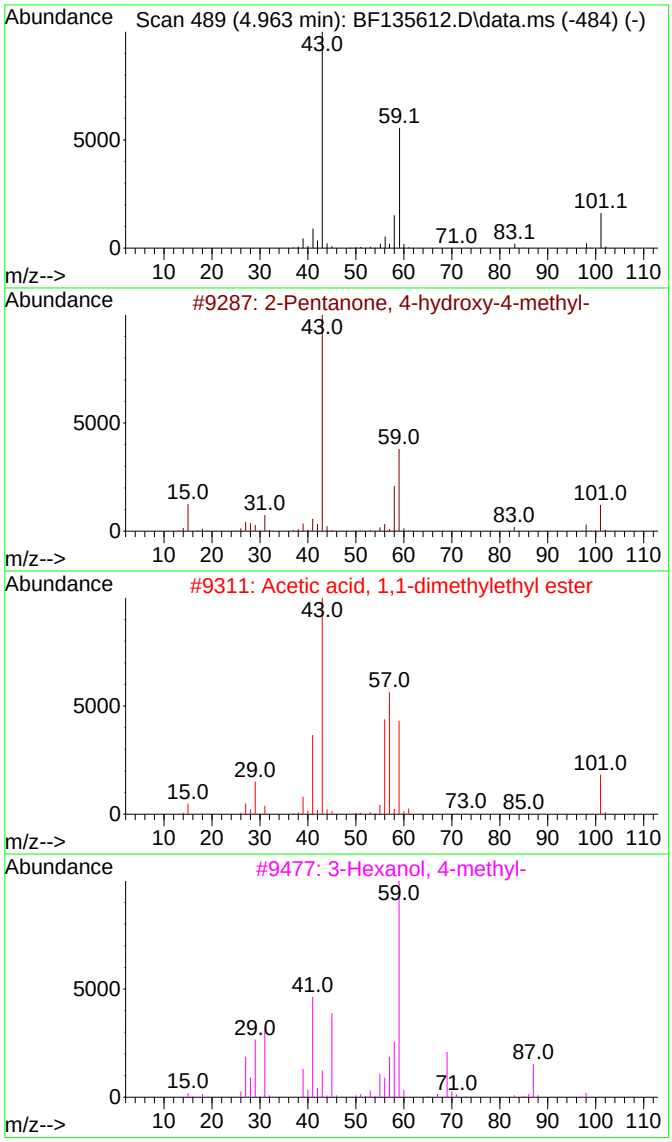
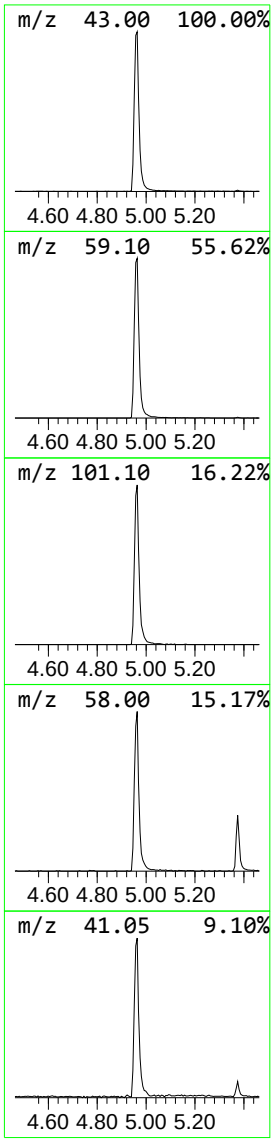
****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	29.07 ng	1242680	1,4-Dichlorobenzene-d4	6.739

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32





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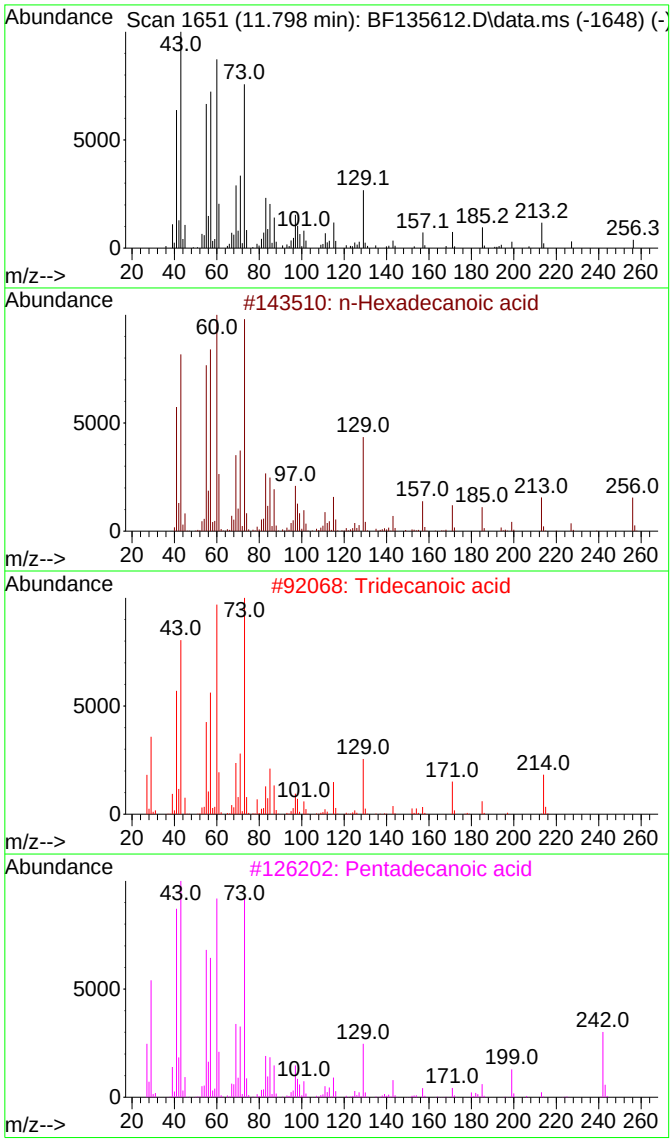
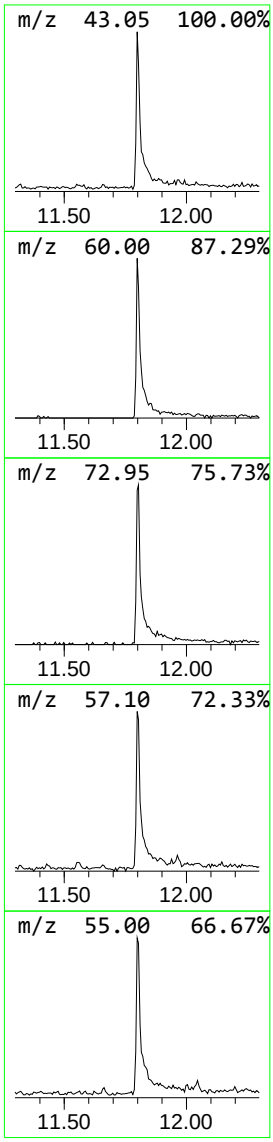
Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.798	6.64 ng	257936	Phenanthrene-d10	11.263

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	90
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	86
5	Undecanoic acid	186	C11H22O2	000112-37-8	72





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Sample : 04714-07
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091123.M
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TIC Library : C:\Database\NIST20.L
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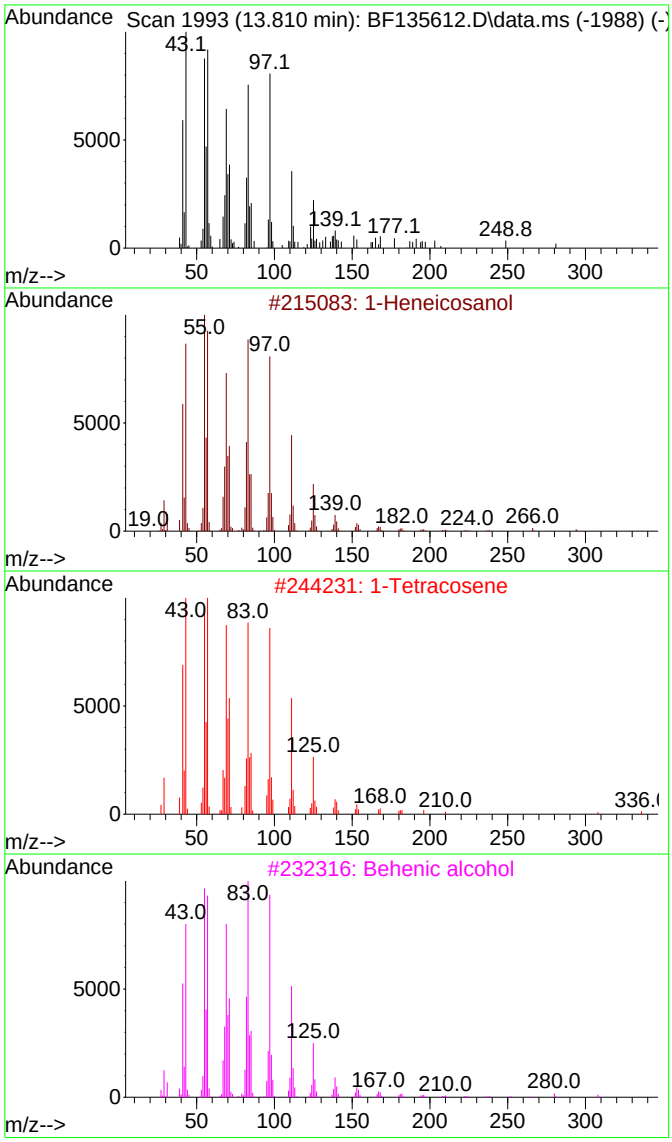
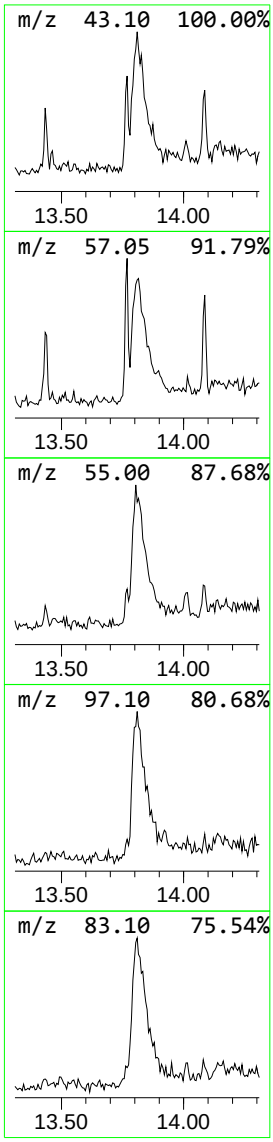
Peak Number 3 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.810	6.26 ng	225485	Chrysene-d12	13.921

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	93
2	1-Tetracosene	336	C24H48	010192-32-2	93
3	Behenic alcohol	326	C22H46O	000661-19-8	93
4	1-Hexacosene	364	C26H52	018835-33-1	93
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	90





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ClientSampleId :
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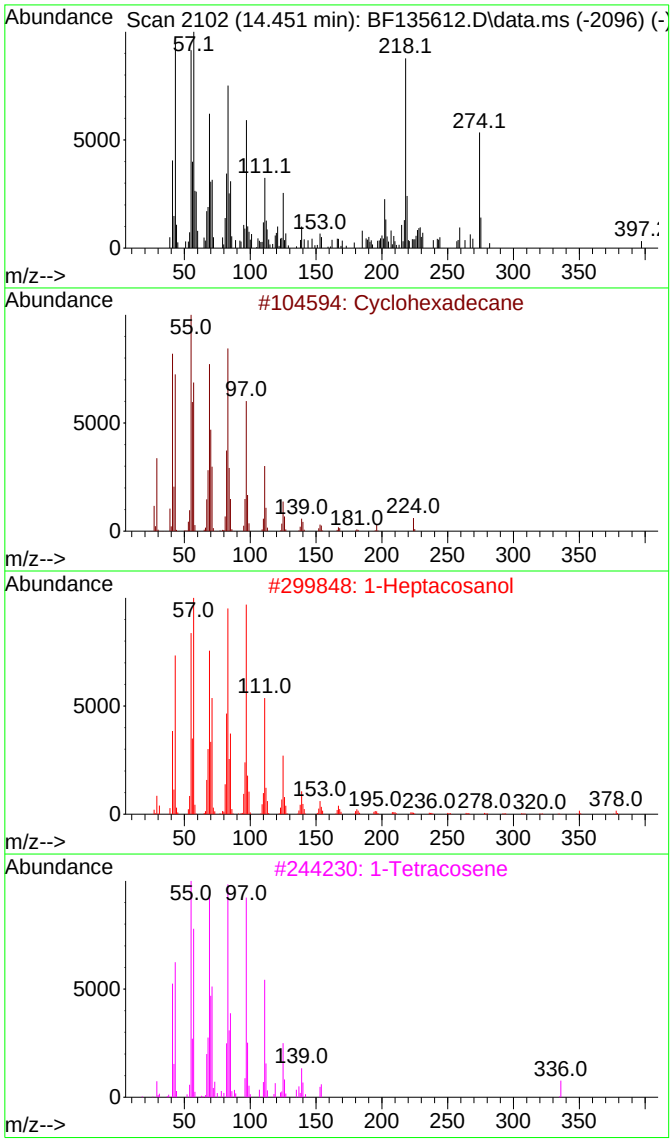
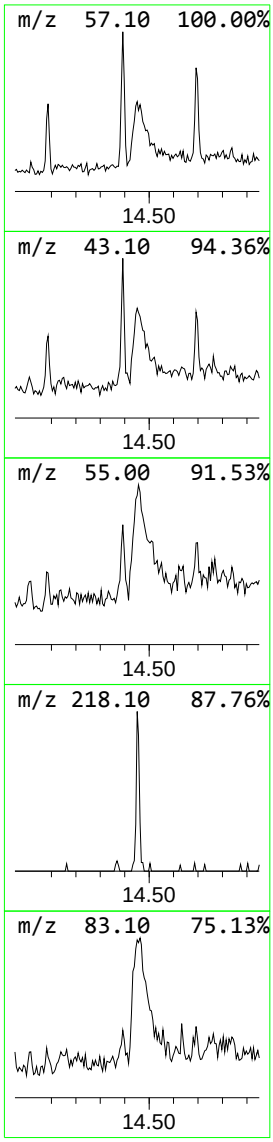
Peak Number 4 Cyclohexadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.451	6.90 ng	248722	Chrysene-d12	13.921

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclohexadecane	224	C16H32	000295-65-8	78
2	1-Heptacosanol	396	C27H56O	002004-39-9	46
3	1-Tetracosene	336	C24H48	010192-32-2	46
4	Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	46
5	Carbonic acid, hexadecyl 2,2,2-t...	416	C19H35Cl3O3	1000314-56-2	46





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TIC Library : C:\Database\NIST20.L
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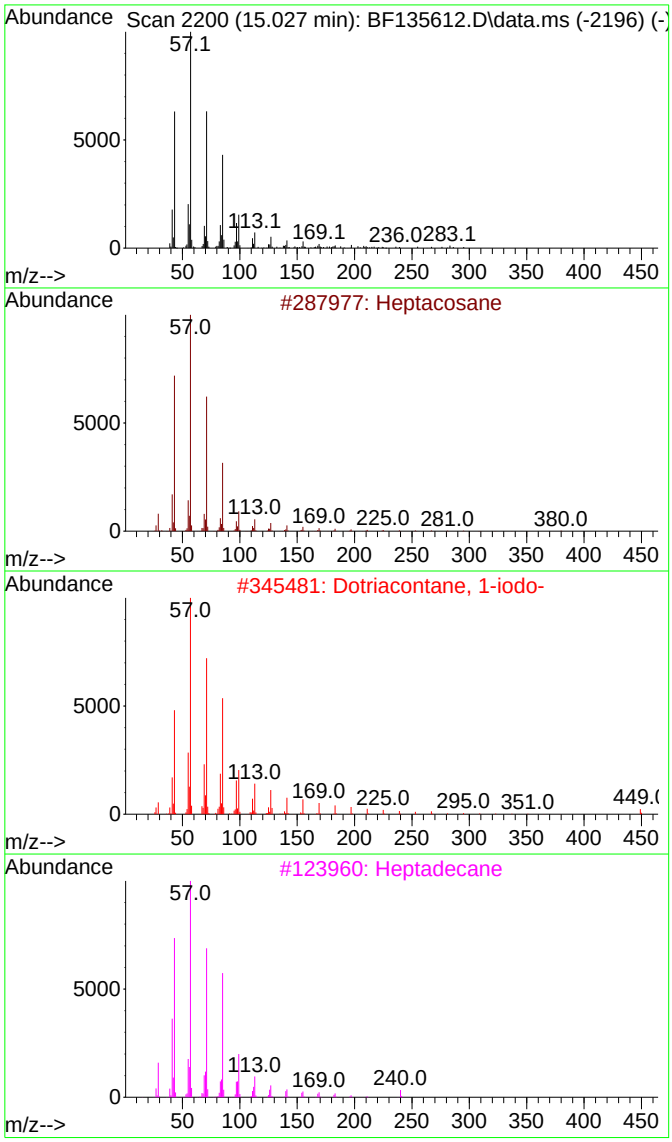
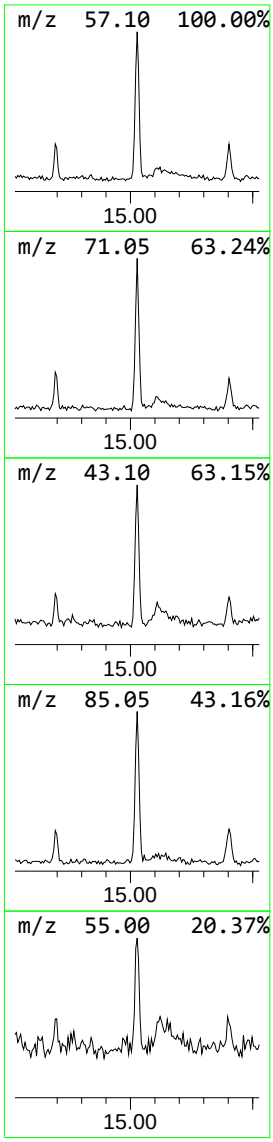
Peak Number 5 Heptacosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.027	4.14 ng	161215	Perylene-d12	15.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
3	Heptadecane	240	C17H36	000629-78-7	90
4	Heneicosane	296	C21H44	000629-94-7	87
5	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	86





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TIC Library : C:\Database\NIST20.L
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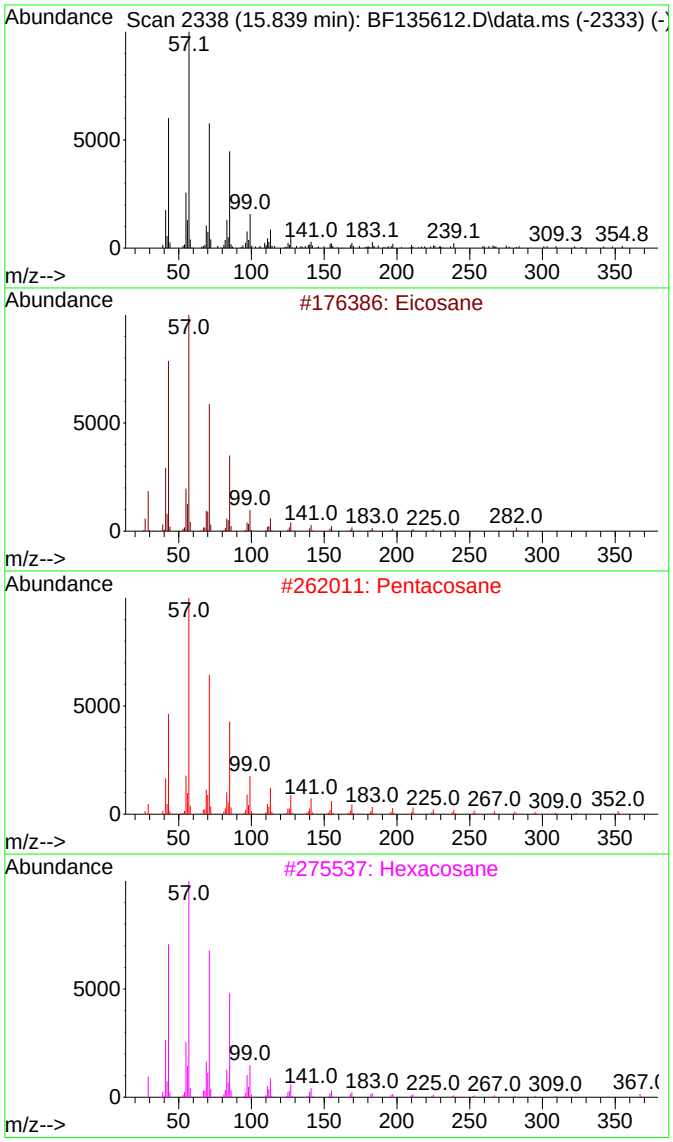
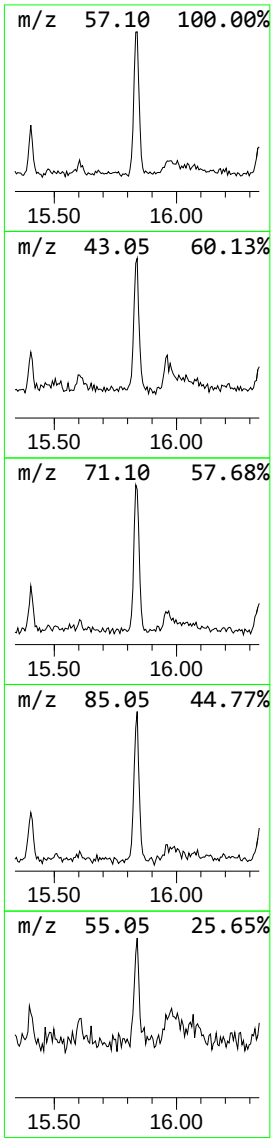
Peak Number 6 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.839	4.08 ng	158675	Perylene-d12	15.392

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	93
2	Pentacosane	352	C25H52	000629-99-2	87
3	Hexacosane	366	C26H54	000630-01-3	87
4	Nonadecane	268	C19H40	000629-92-5	87
5	Docosane	310	C22H46	000629-97-0	87





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-...	4.963	29.1	ng	1242680	1	6.739	855011	20.0
n-Hexadecanoic ...	11.798	6.6	ng	257936	4	11.263	777049	20.0
1-Heneicosanol	13.810	6.3	ng	225485	5	13.921	720539	20.0
Cyclohexadecane	14.451	6.9	ng	248722	5	13.921	720539	20.0
Heptacosane	15.027	4.1	ng	161215	6	15.392	778451	20.0
Eicosane	15.839	4.1	ng	158675	6	15.392	778451	20.0