LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP040721\
Data File : BP005216.D
Acq On : 07 Apr 2021 12:32
Operator : CG/JU
Sample : M1933-12
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : BENNETT_BH_04_2-2.5

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_P\Methods\8270E-BP032321.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP005216.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.834	294	297	305	rVB3	8803	14541	1.71%	0.294%
2	5.293	369	375	383	rBV	292205	411793	48.54%	8.316%
3	6.875	635	644	653	rBV	266992	426077	50.23%	8.605%
4	7.693	776	783	790	rVB	71045	115962	13.67%	2.342%
5	8.852	973	980	989	rBV	162788	268744	31.68%	5.427%
6	10.481	1249	1257	1264	rBV	95434	158568	18.69%	3.202%
7	12.963	1671	1679	1686	rBV	377922	555722	65.51%	11.223%
8	13.810	1818	1823	1830	rVB	15098	23119	2.73%	0.467%
9	14.345	1907	1914	1921	rBV2	134523	204057	24.06%	4.121%
10	15.845	2160	2169	2180	rBV	268347	400602	47.23%	8.090%
11	17.110	2375	2384	2389	rBV	167960	243259	28.68%	4.913%
12	17.151	2389	2391	2395	rVB2	9971	11339	1.34%	0.229%
13	18.010	2529	2537	2545	rBV2	107330	157727	18.59%	3.185%
14	18.475	2611	2616	2622	rBV6	5299	13444	1.58%	0.272%
15	18.580	2630	2634	2638	rBV4	7553	9605	1.13%	0.194%
16	18.739	2657	2661	2665	rBV2	27263	30878	3.64%	0.624%
17	19.016	2703	2708	2714	rBV8	5520	11058	1.30%	0.223%
18	19.133	2720	2728	2734	rBV2	52599	79981	9.43%	1.615%
19	19.245	2742	2747	2757	rBV2	48644	86410	10.19%	1.745%
20	19.480	2784	2787	2791	rVB	29443	37319	4.40%	0.754%
21	19.686	2816	2822	2830	rBV	694173	848272	100.00%	17.131%
22	19.798	2838	2841	2847	rVB8	5724	10068	1.19%	0.203%
23	20.345	2931	2934	2938	rBV4	8216	11409	1.34%	0.230%
24	20.545	2965	2968	2974	rBV	30720	37020	4.36%	0.748%
25	20.874	3022	3024	3027	rVB4	11995	10422	1.23%	0.210%
26	20.921	3028	3032	3040	rVB	84076	115671	13.64%	2.336%
27	21.204	3075	3080	3085	rBV	236756	324483	38.25%	6.553%
28	22.786	3345	3349	3353	rBV4	23298	49620	5.85%	1.002%
29	23.486	3462	3468	3475	rVB2	158477	284459	33.53%	5.745%

Sum of corrected areas: 4951629

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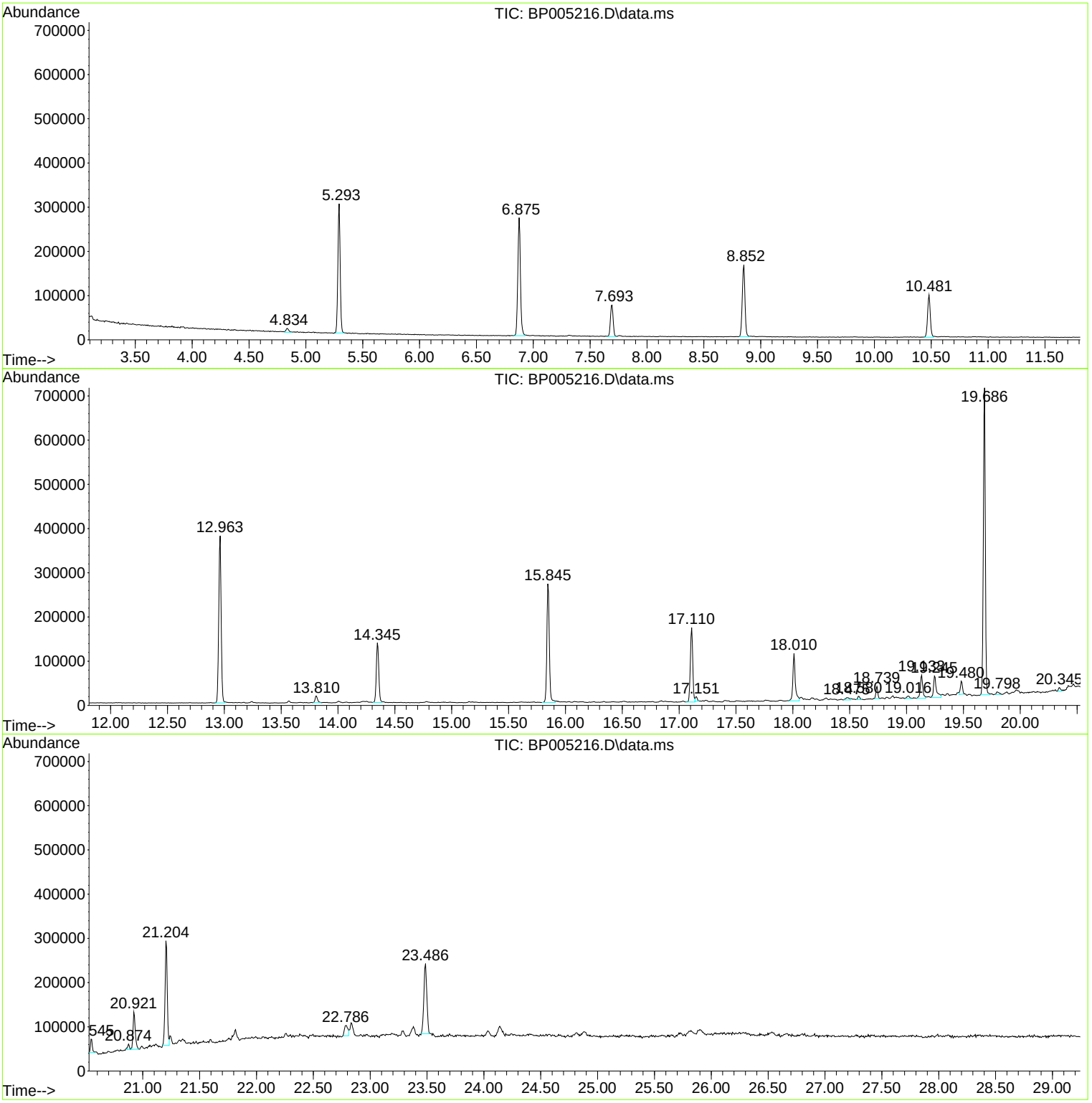
Instrument :
BNA_P
ClientSampleId :
BENNETT_BH_04_2-2.5

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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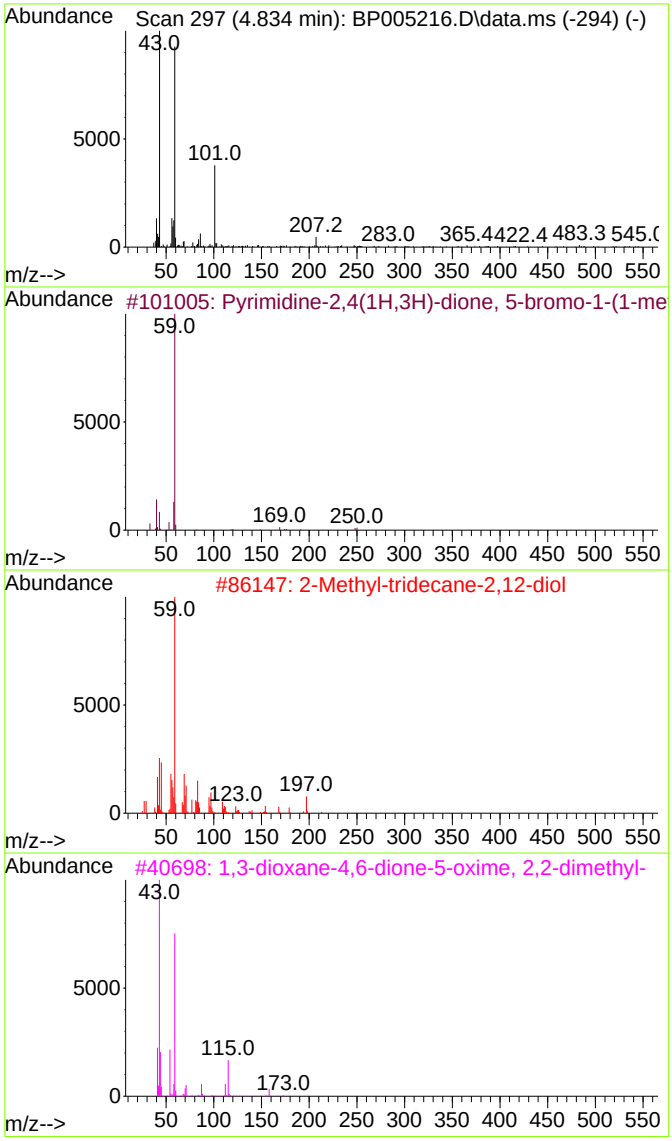
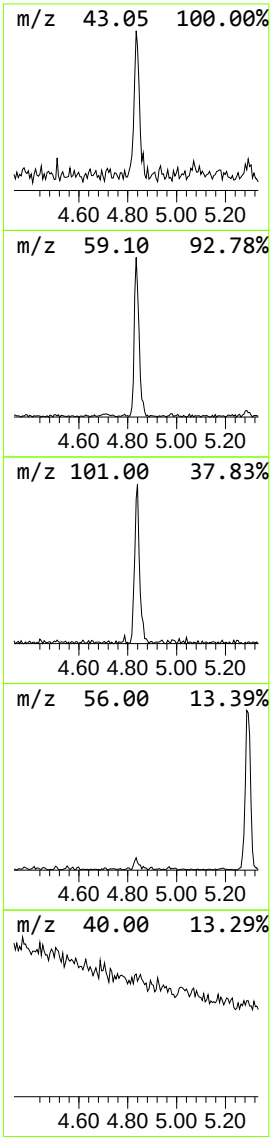
****
Peak Number 1 Pyrimidine-2,4(1H,3H)-dione... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.834	2.51 ng	14541	1,4-Dichlorobenzene-d4	7.693

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pyrimidine-2,4(1H,3H)-dione, 5-b...	248	C7H9BrN2O3	296879-03-3	50
2	2-Methyl-tridecane-2,12-diol	230	C14H30O2	1000187-03-5	40
3	1,3-dioxane-4,6-dione-5-oxime, 2...	173	C6H7NO5	081539-54-0	40
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	39
5	3-Heptanol, 5-methyl-	130	C8H18O	018720-65-5	38





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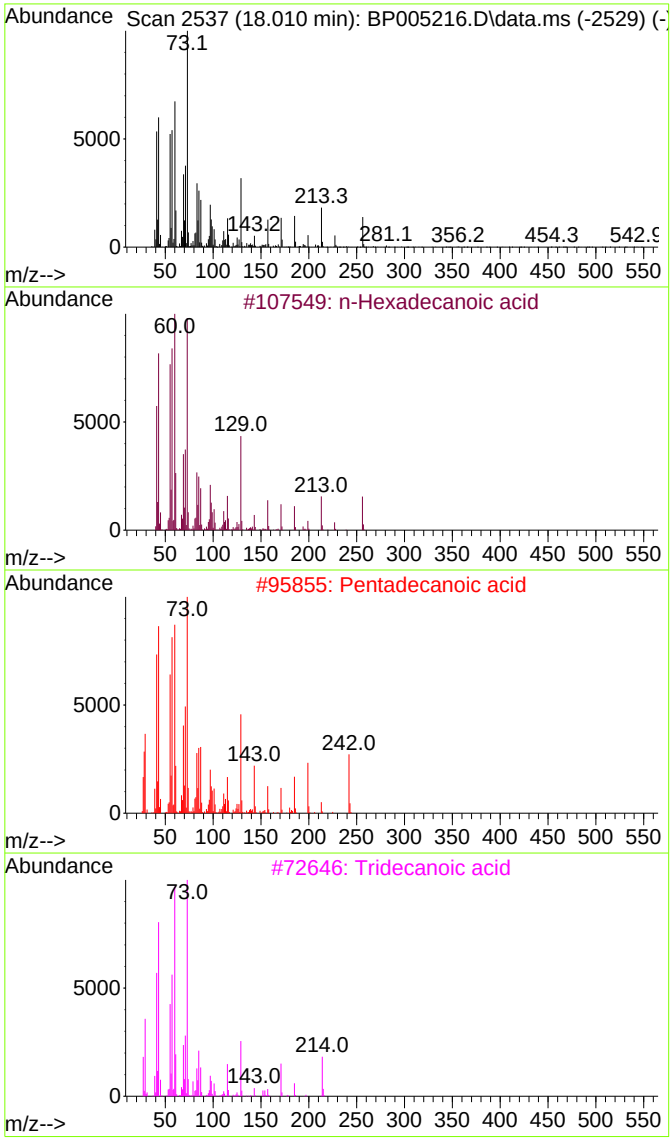
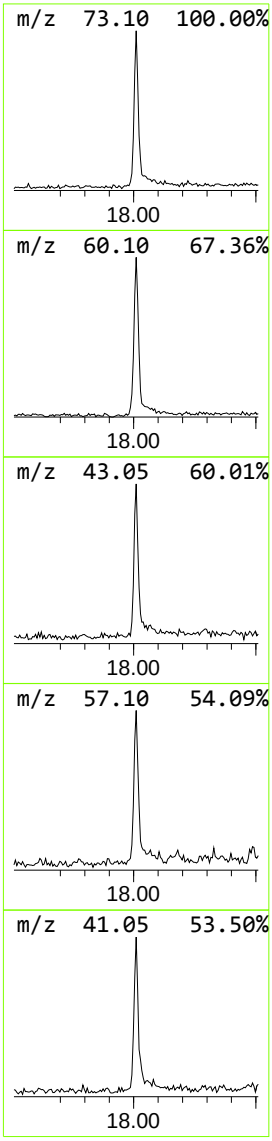
****
Peak Number 2 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.010	12.97 ng	157727	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
3	Tridecanoic acid	214	C13H26O2	000638-53-9	52
4	n-Decanoic acid	172	C10H20O2	000334-48-5	43
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	35





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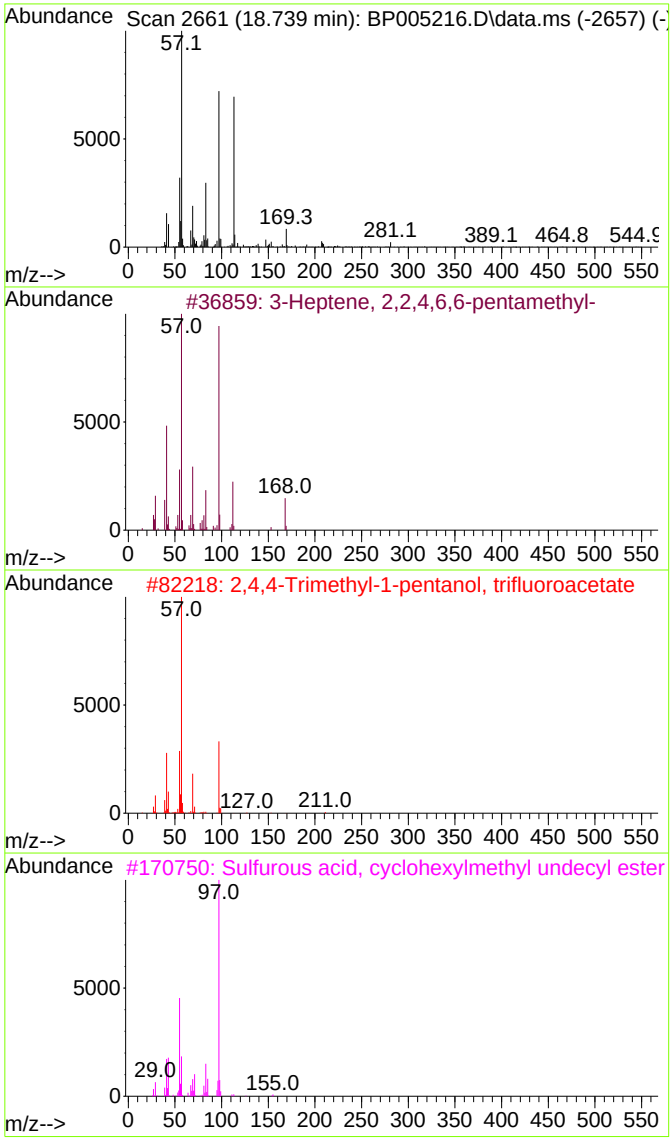
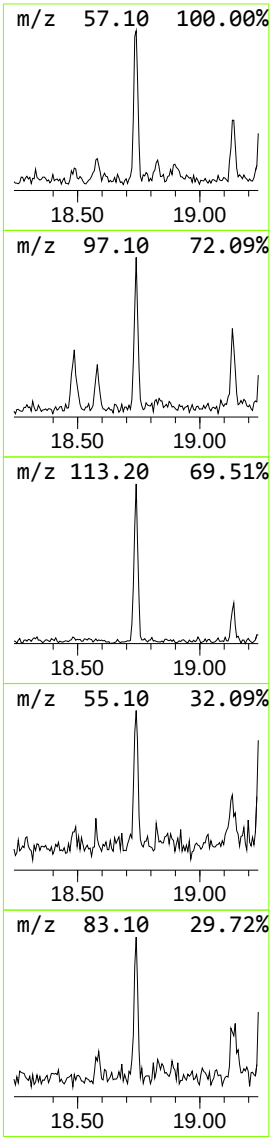
****

Peak Number 3 unknown18.73 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.739	2.54 ng	30878	Phenanthrene-d10	17.110

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Heptene, 2,2,4,6,6-pentamethyl-	168	C12H24	000123-48-8	32
2	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	27
3	Sulfurous acid, cyclohexylmethyl...	332	C18H36O3S	1000309-21-9	27
4	5-Nonanone, 2,2,8,8-tetramethyl-	198	C13H26O	005709-95-5	25
5	1-Ethyl-3-methylcyclohexane (c,t)	126	C9H18	003728-55-0	18





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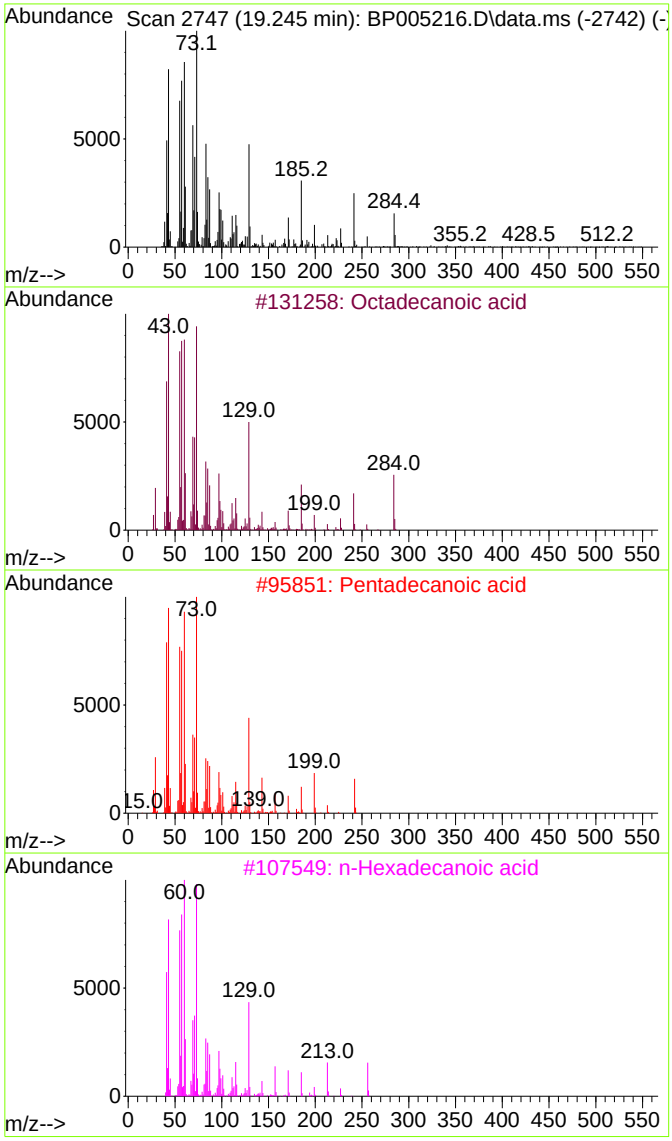
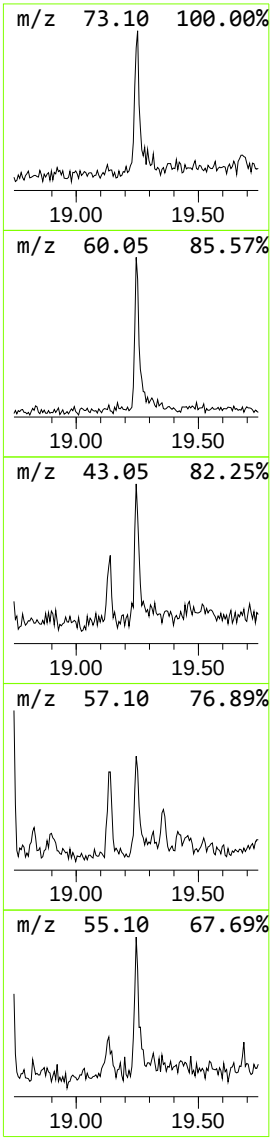
****

Peak Number 4 Octadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.245	5.33 ng	86410	Chrysene-d12	21.204

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	74
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	52
5	11-Bromoundecanoic acid	264	C11H21BrO2	002834-05-1	50





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Instrument :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP032321.M
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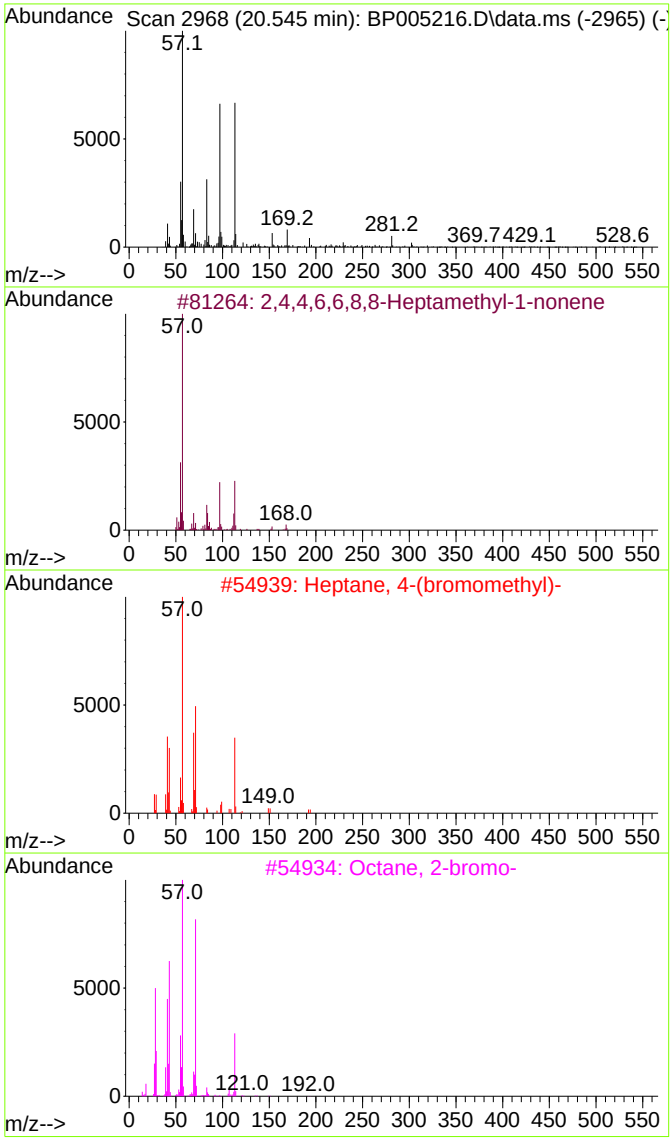
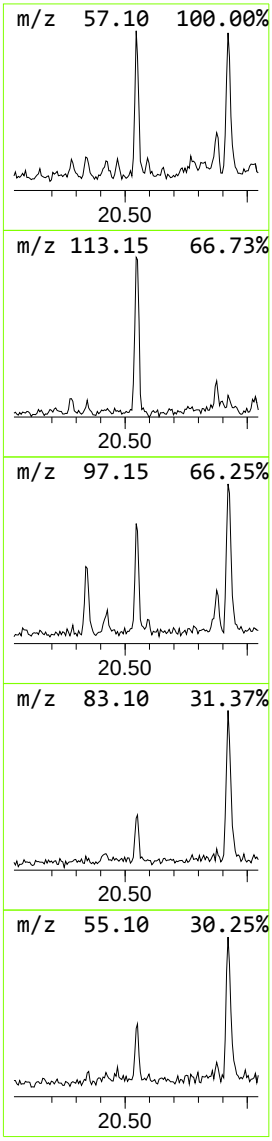
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 2,4,4,6,6,8,8-Heptamethyl-1... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.545	2.28 ng	37020	Chrysene-d12	21.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,4,6,6,8,8-Heptamethyl-1-nonene	224	C16H32	015796-04-0	59
2	Heptane, 4-(bromomethyl)-	192	C8H17Br	101654-29-9	35
3	Octane, 2-bromo-	192	C8H17Br	000557-35-7	35
4	2,4,4-Trimethyl-1-pentanol, trif...	226	C10H17F3O2	1000365-19-5	27
5	Cyclohexane, (bromomethyl)-	176	C7H13Br	002550-36-9	27





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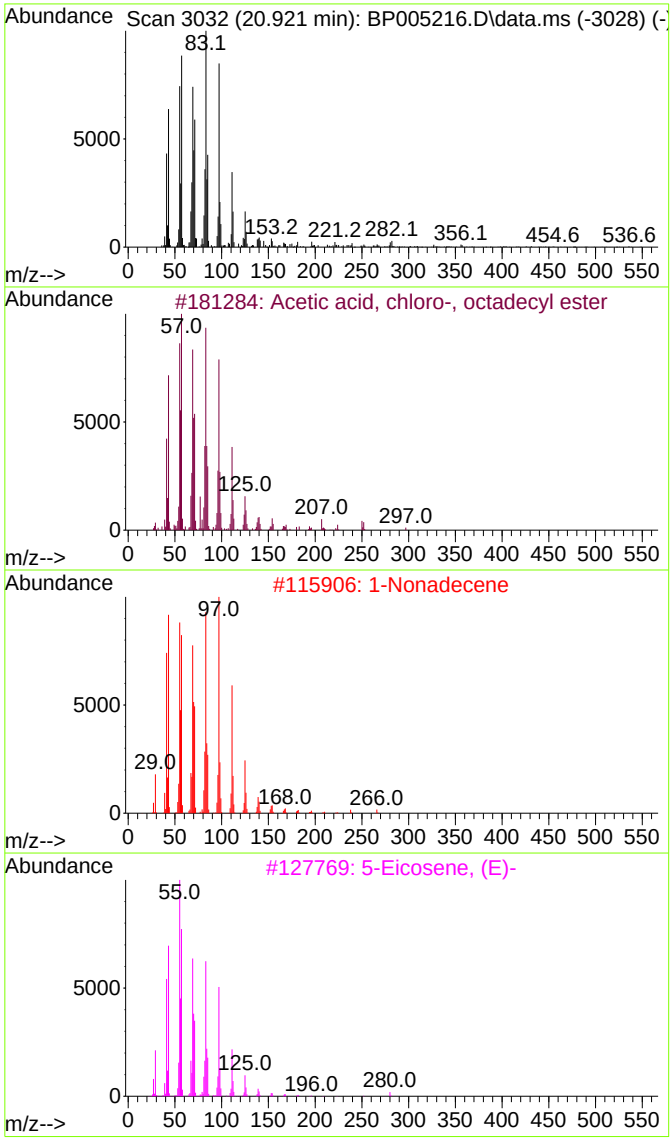
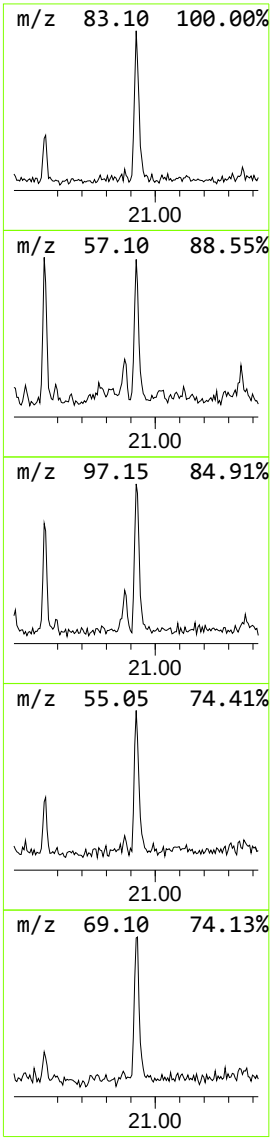
****
Peak Number 6 Acetic acid, chloro-, octad... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.922	7.13 ng	115671	Chrysene-d12	21.204

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetic acid, chloro-, octadecyl ...	346	C20H39ClO2	005348-82-3	91
2	1-Nonadecene	266	C19H38	018435-45-5	90
3	5-Eicosene, (E)-	280	C20H40	074685-30-6	89
4	Cyclotetradecane	196	C14H28	000295-17-0	89
5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	87





Tentatively Identified Compound (LSC) summary

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					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Pyrimidine-2,4(...	4.834	2.5	ng	14541	1	7.693	115962	20.0
n-Hexadecanoic ...	18.010	13.0	ng	157727	4	17.110	243259	20.0
unknown18.73	18.739	2.5	ng	30878	4	17.110	243259	20.0
Octadecanoic acid	19.245	5.3	ng	86410	5	21.204	324483	20.0
2,4,4,6,6,8,8-H...	20.545	2.3	ng	37020	5	21.204	324483	20.0
Acetic acid, ch...	20.922	7.1	ng	115671	5	21.204	324483	20.0