LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP091922\
Data File : BP011750.D
Acq On : 19 Sep 2022 23:53
Operator : CG/JU
Sample : N4684-01
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : 5486-2

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-BP091422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP011750.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.070	9	14	30	rVB	12741902	19030628	72.32%	14.579%
2	5.028	341	347	361	rBV2	211721	350379	1.33%	0.268%
3	5.493	417	426	441	rBV	4347542	6639365	25.23%	5.086%
4	7.093	690	698	718	rBV	3311815	5306941	20.17%	4.066%
5	7.934	833	841	848	rBV	1313492	2110122	8.02%	1.617%
6	9.099	1032	1039	1053	rBV	4228478	7127946	27.09%	5.461%
7	10.746	1310	1319	1332	rBV	1934646	3290997	12.51%	2.521%
8	11.657	1467	1474	1489	rBV	113371	287145	1.09%	0.220%
9	13.199	1729	1736	1751	rBV	11336127	17371963	66.02%	13.309%
10	14.575	1962	1970	1980	rBV	3251905	4732530	17.98%	3.626%
11	14.993	2034	2041	2065	rBV	826658	1571057	5.97%	1.204%
12	16.063	2212	2223	2243	rBV	9353963	13309442	50.58%	10.196%
13	16.722	2330	2335	2345	rBV	237208	425854	1.62%	0.326%
14	17.322	2431	2437	2450	rVB	3921257	5793007	22.01%	4.438%
15	18.204	2583	2587	2597	rBV	700962	1234206	4.69%	0.946%
16	19.439	2792	2797	2809	rBV2	334883	676733	2.57%	0.518%
17	19.692	2836	2840	2851	rBV	364296	577025	2.19%	0.442%
18	19.875	2866	2871	2877	rBV	19838993	26314732	100.00%	20.160%
19	21.110	3077	3081	3093	rBV	912542	1482924	5.64%	1.136%
20	21.404	3126	3131	3140	rBV	4914590	6484612	24.64%	4.968%
21	23.851	3541	3547	3559	rVB2	3128752	6413467	24.37%	4.913%

Sum of corrected areas: 130531075

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Misc :
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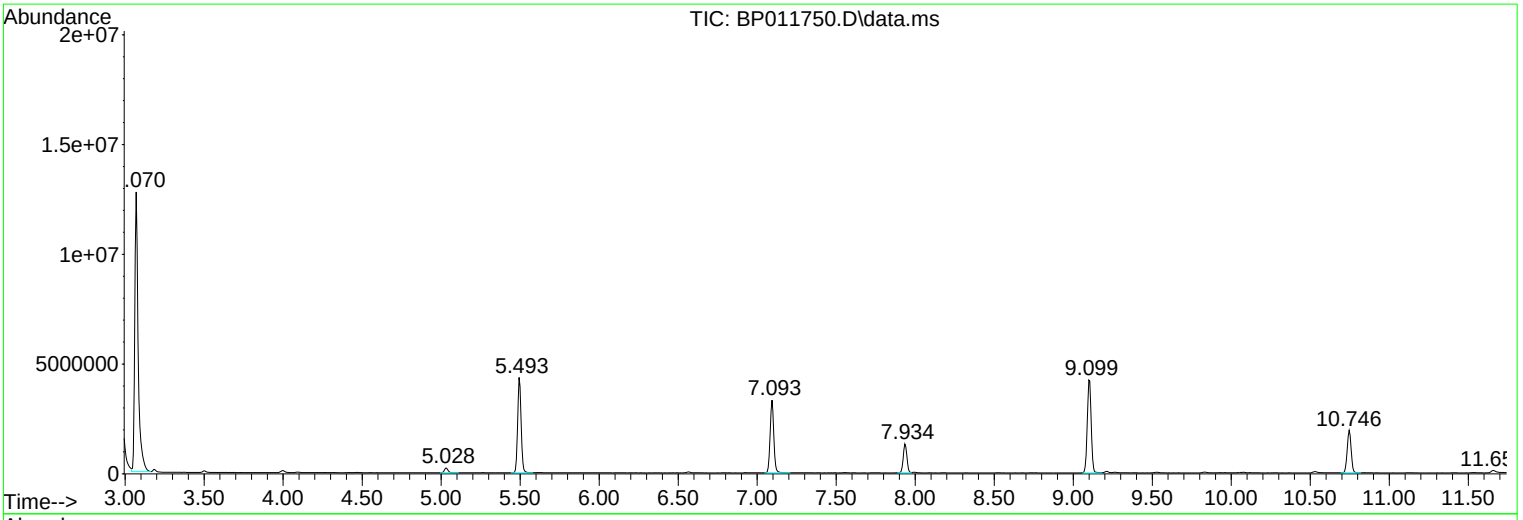
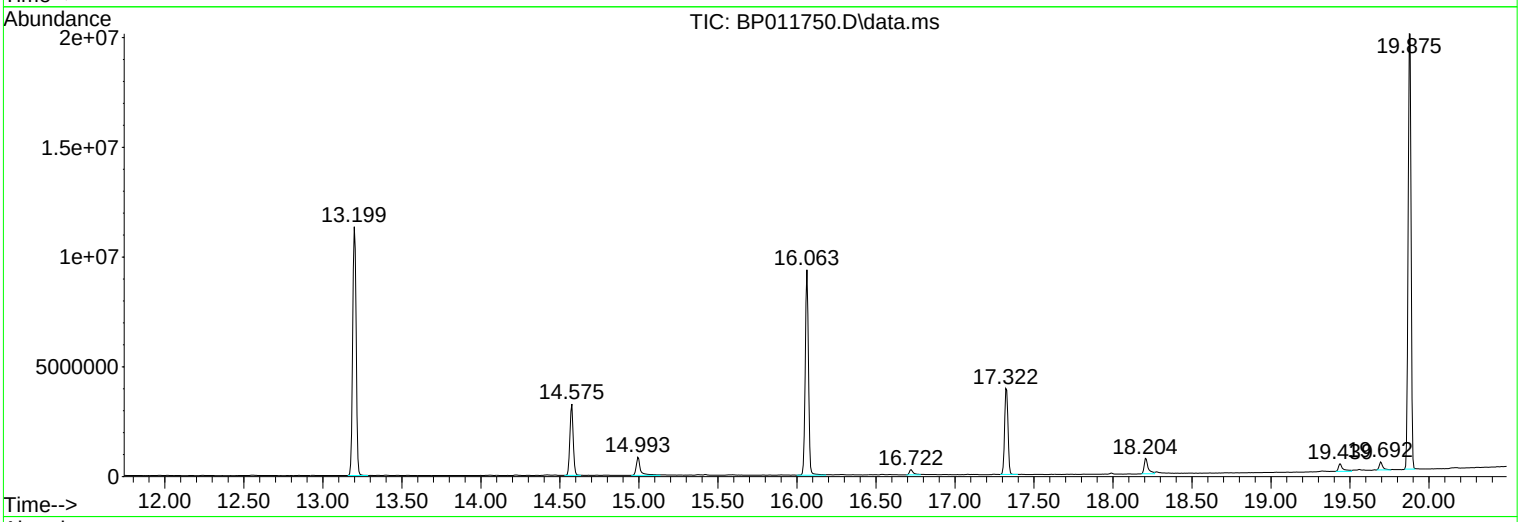
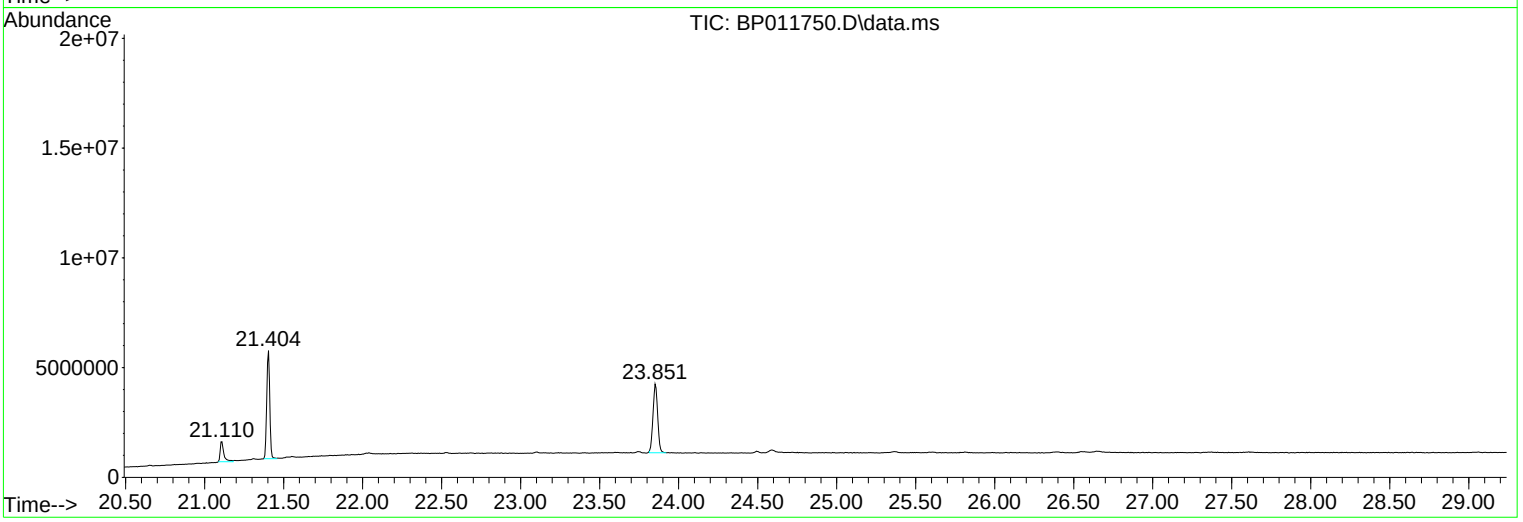
Instrument :
BNA_P
ClientSampleId :
5486-2

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091422.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

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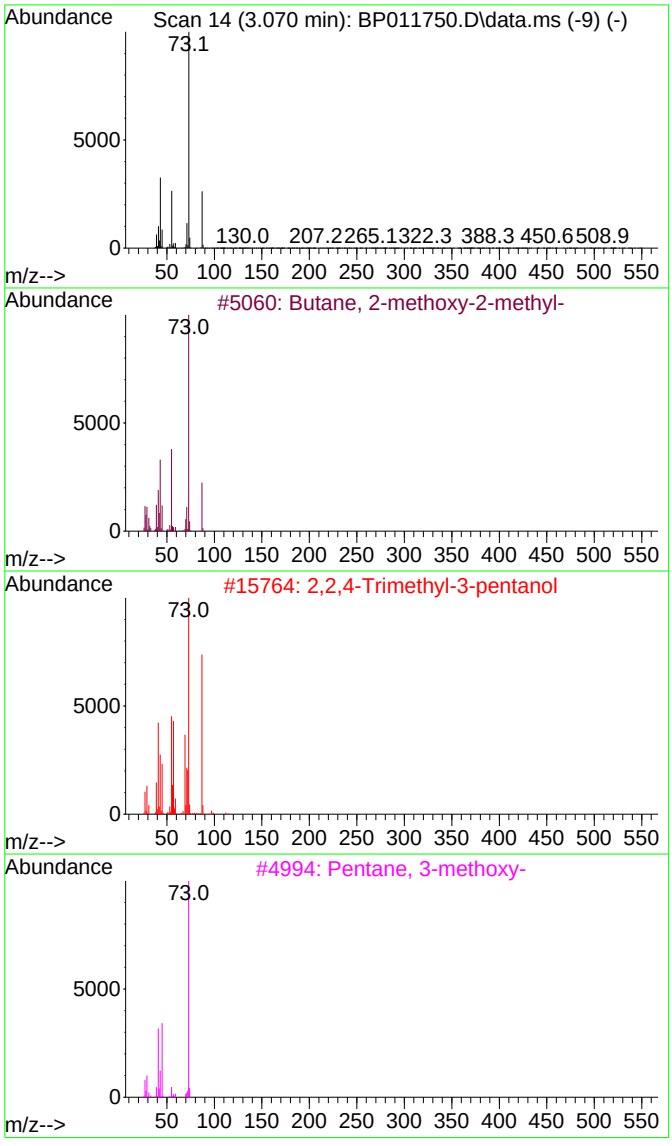
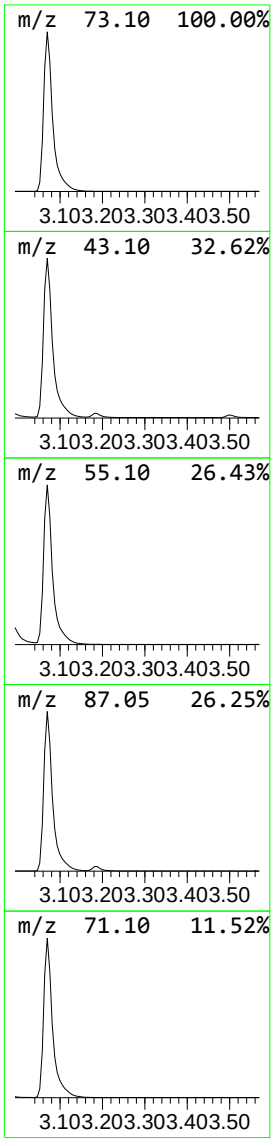
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.070	180.38 ng	19030600	1,4-Dichlorobenzene-d4	7.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
4	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5	N-Ethylformamide	73	C3H7NO	000627-45-2	9





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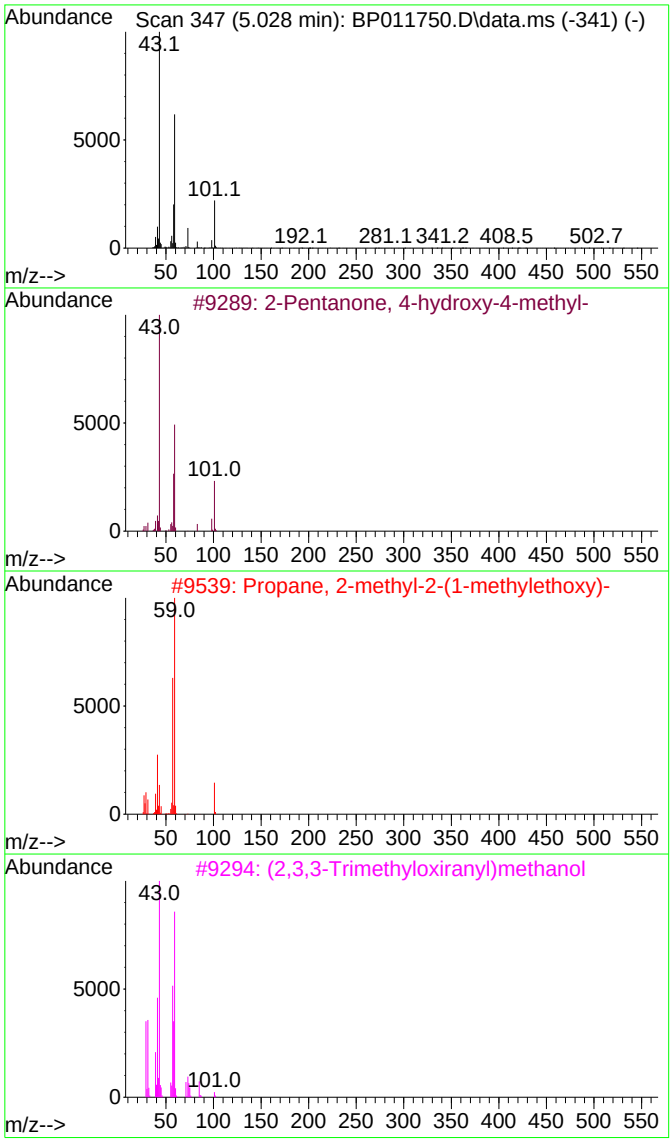
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

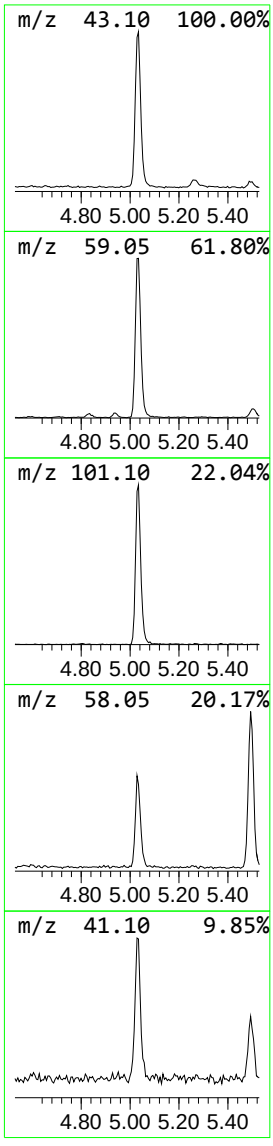
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.028	3.32 ng	350379	1,4-Dichlorobenzene-d4	7.934

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	37
3	(2,3,3-Trimethyloxiranyl)methanol	116	C6H12O2	1000306-64-7	36
4	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	33
5	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25





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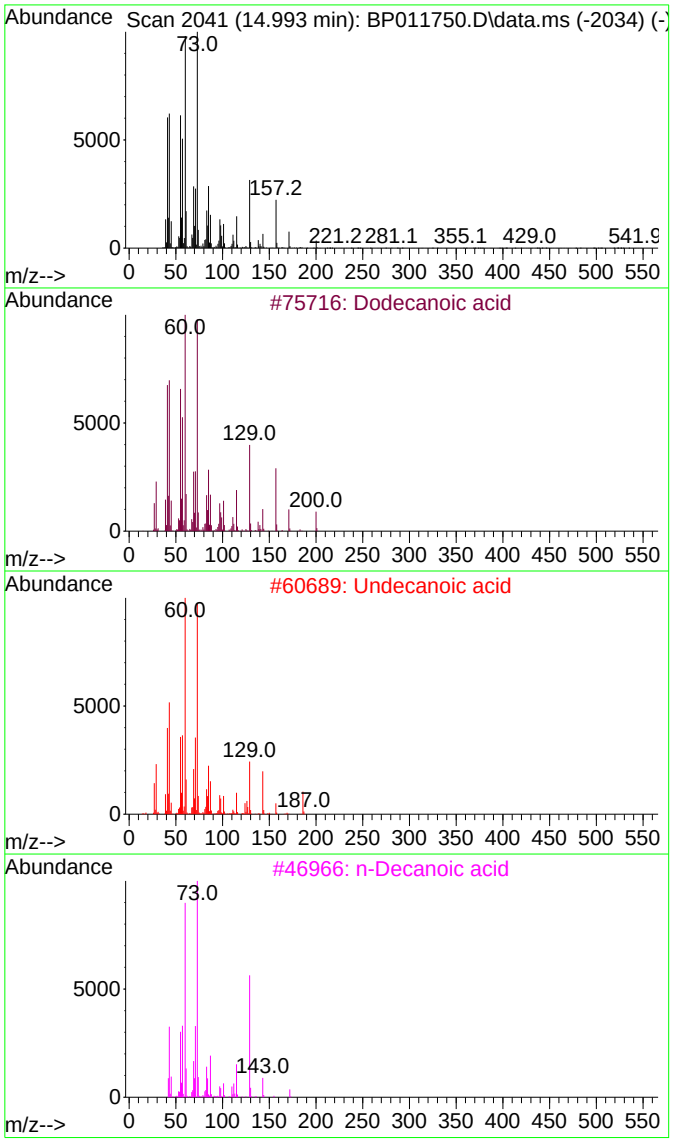
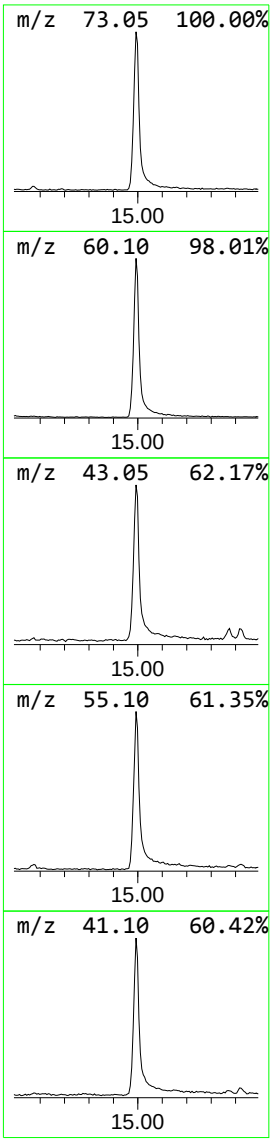
****

Peak Number 3 Dodecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.993	6.64 ng	1571060	Acenaphthene-d10	14.575

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dodecanoic acid	200	C12H24O2	000143-07-7	98
2	Undecanoic acid	186	C11H22O2	000112-37-8	78
3	n-Decanoic acid	172	C10H20O2	000334-48-5	70
4	Nonanoic acid	158	C9H18O2	000112-05-0	62
5	Hexanoic acid	116	C6H12O2	000142-62-1	35





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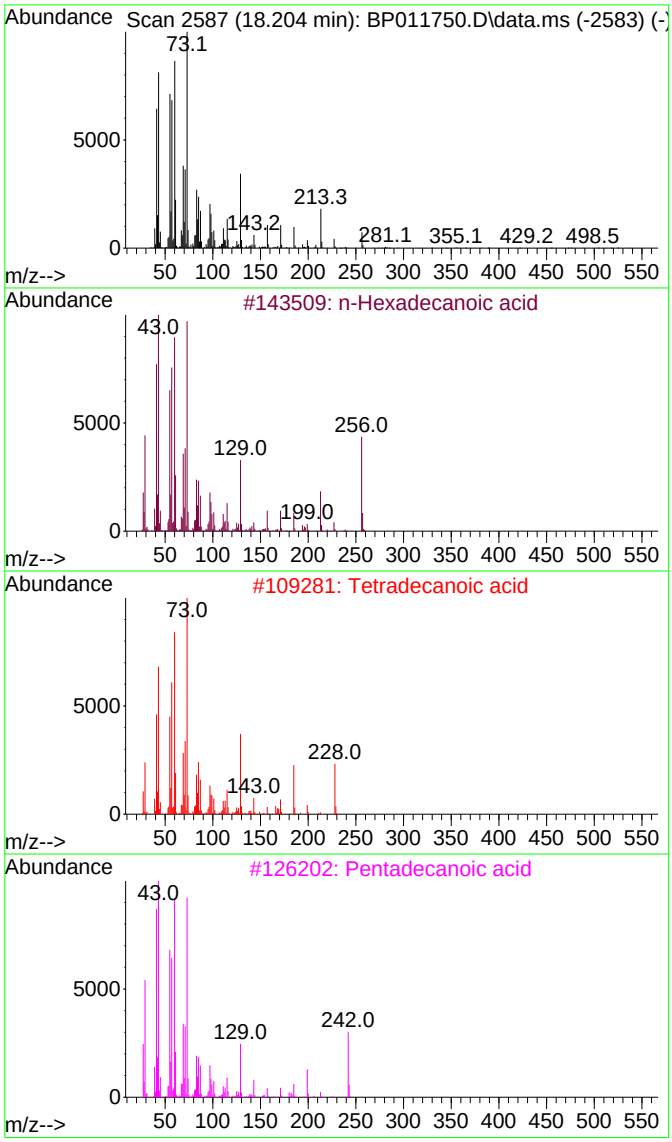
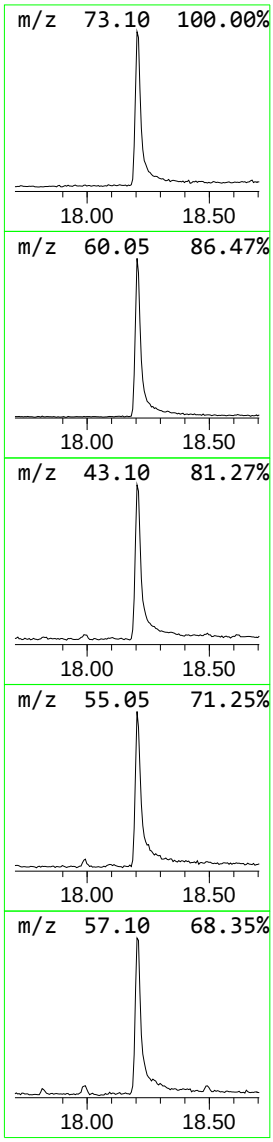
****

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.204	4.26 ng	1234210	Phenanthrene-d10	17.322

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	93
4	Tridecanoic acid	214	C13H26O2	000638-53-9	81
5	Isopropyl palmitate	298	C19H38O2	000142-91-6	59





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Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\8270E-BP091422.M
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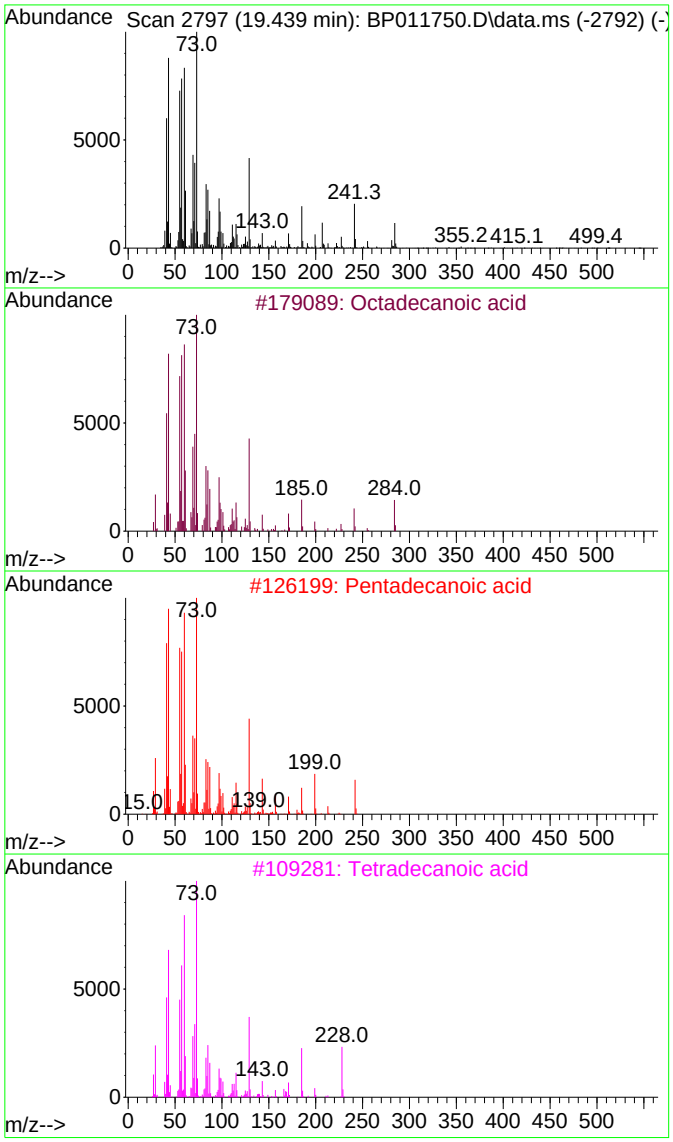
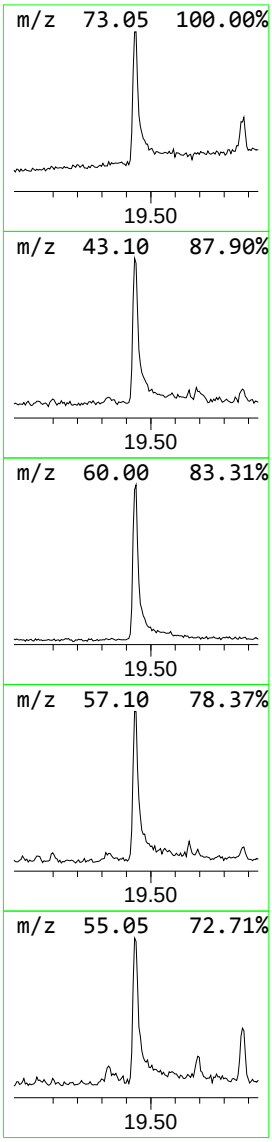
****

Peak Number 5 Octadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.439	2.09 ng	676733	Chrysene-d12	21.404

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	91
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	59





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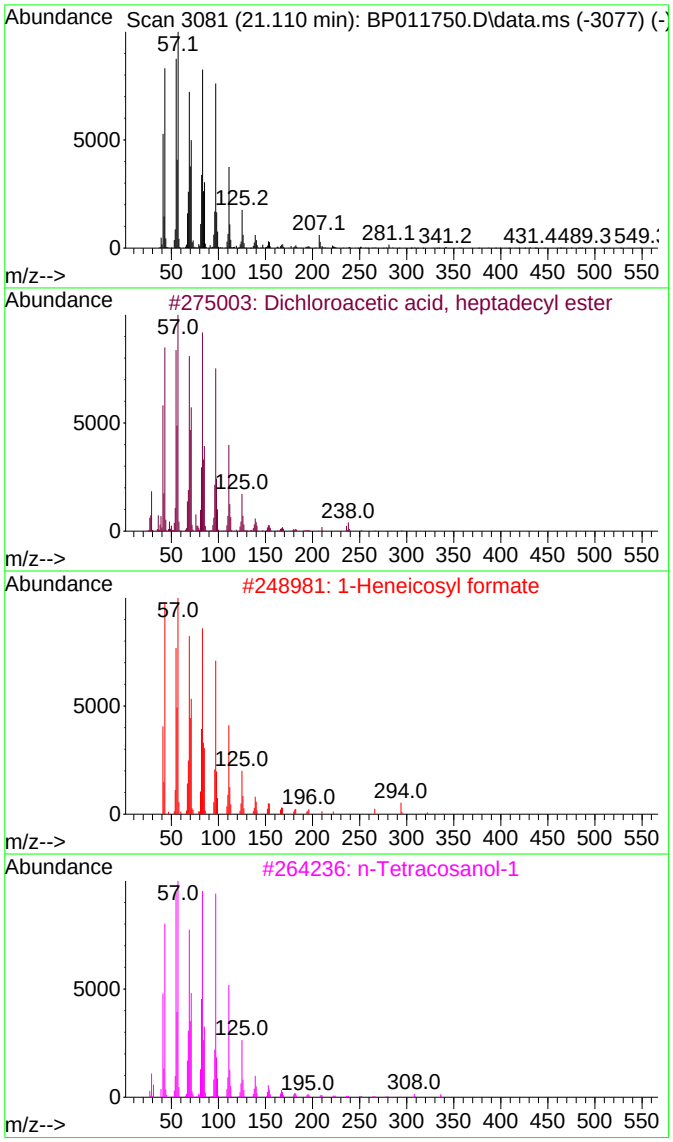
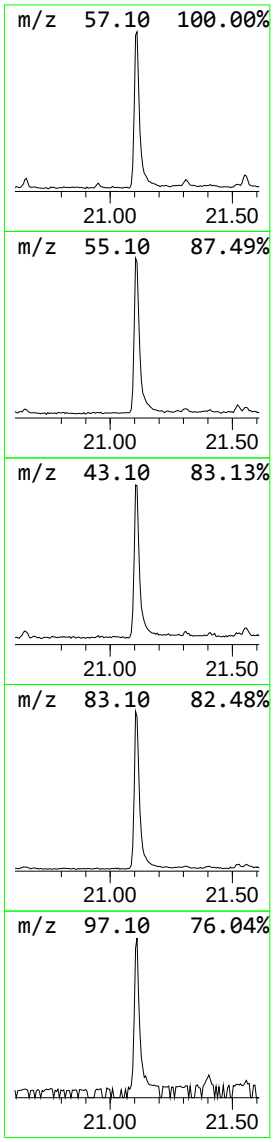
****
Peak Number 6 Dichloroacetic acid, heptad... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.110	4.57 ng	1482920	Chrysene-d12	21.404

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
2	1-Heneicosyl formate	340	C22H44O2	077899-03-7	94
3	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	94
5	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94





Tentatively Identified Compound (LSC) summary

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					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	3.070	180.4	ng	19030600	1	7.934	2110120	20.0
2-Pentanone, 4-...	5.028	3.3	ng	350379	1	7.934	2110120	20.0
Dodecanoic acid	14.993	6.6	ng	1571060	3	14.575	4732530	20.0
n-Hexadecanoic ...	18.204	4.3	ng	1234210	4	17.322	5793010	20.0
Octadecanoic acid	19.439	2.1	ng	676733	5	21.404	6484610	20.0
Dichloroacetic ...	21.110	4.6	ng	1482920	5	21.404	6484610	20.0