LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128675.D
Acq On : 03 Jun 2022 12:46
Operator : CG\JU
Sample : N3025-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : UST-BOT

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-BF060222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF128675.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.357	179	182	191	rBV	32842	61591	2.17%	0.333%
2	5.045	465	469	474	rVB	23124	28833	1.02%	0.156%
3	5.469	538	541	550	rBV	2375628	2336947	82.52%	12.636%
4	6.481	710	713	724	rBV	2368340	2393534	84.52%	12.942%
5	6.563	724	727	730	rVB	48548	32987	1.16%	0.178%
6	6.822	767	771	774	rBV	703950	540403	19.08%	2.922%
7	7.386	861	867	870	rBV	1692322	1626683	57.44%	8.796%
8	8.104	984	989	992	rBV	849861	684275	24.16%	3.700%
9	9.186	1167	1173	1176	rBV	2932347	2831957	100.00%	15.313%
10	9.445	1212	1217	1224	rBV	39614	35595	1.26%	0.192%
11	9.863	1283	1288	1291	rVB	872491	770270	27.20%	4.165%
12	10.651	1418	1422	1426	rBV	1956848	1884212	66.53%	10.188%
13	11.345	1537	1540	1544	rVB	839932	765529	27.03%	4.139%
14	11.745	1605	1608	1610	rBV	120628	101612	3.59%	0.549%
15	11.880	1627	1631	1639	rBV3	154409	169171	5.97%	0.915%
16	12.451	1725	1728	1731	rVB	122201	95589	3.38%	0.517%
17	12.539	1740	1743	1747	rVB	50430	45043	1.59%	0.244%
18	12.668	1761	1765	1774	rVB2	75335	89960	3.18%	0.486%
19	12.939	1806	1811	1814	rBV	2855132	2355049	83.16%	12.734%
20	13.886	1967	1972	1984	rVB5	32618	94712	3.34%	0.512%
21	13.992	1985	1990	1993	rBV	551670	498608	17.61%	2.696%
22	14.086	2001	2006	2015	rVB	332058	348069	12.29%	1.882%
23	14.362	2038	2053	2054	rBV7	91912	258861	9.14%	1.400%
24	15.451	2234	2238	2243	rBV	358225	444143	15.68%	2.402%

Sum of corrected areas: 18493633

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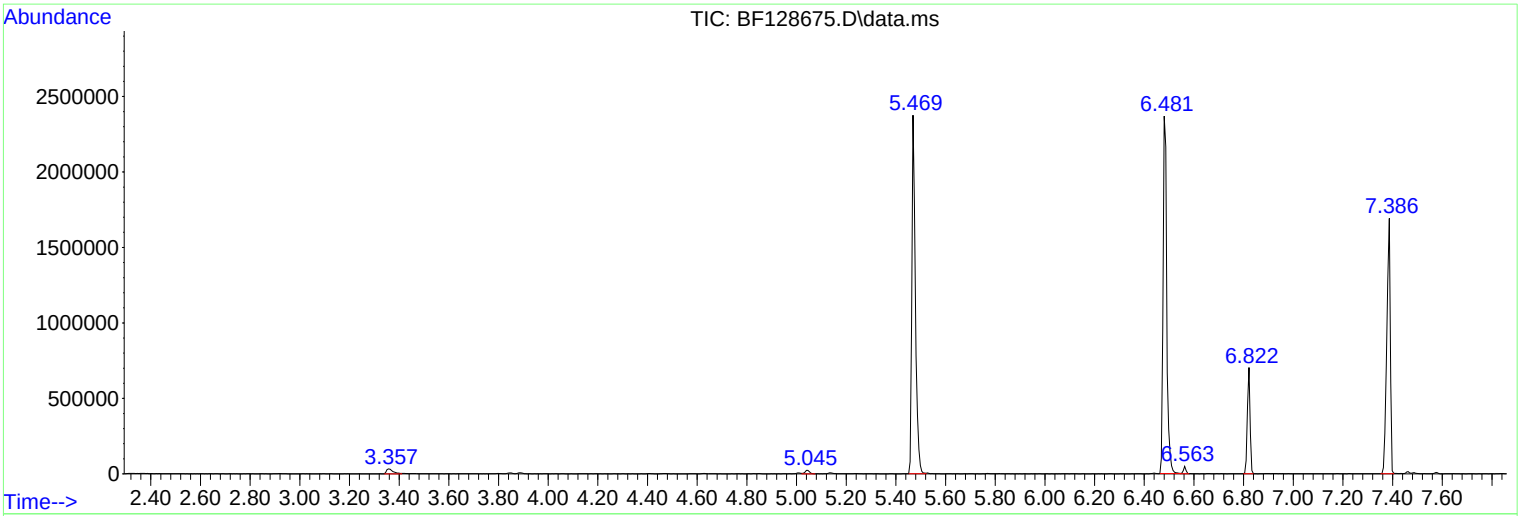
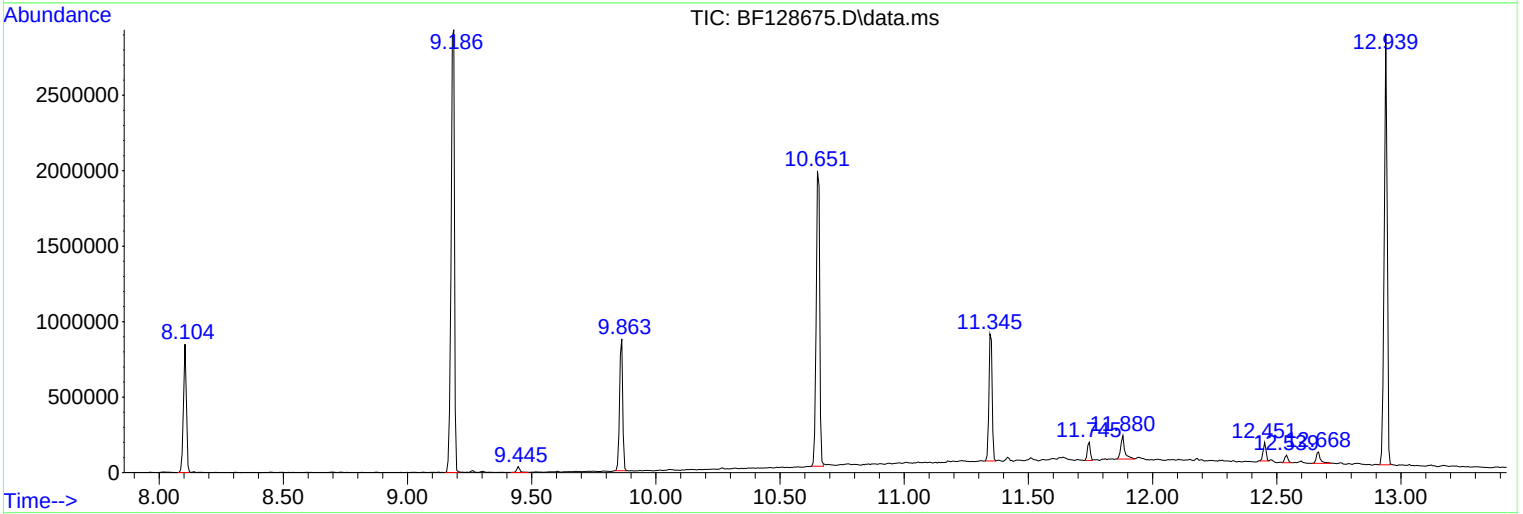
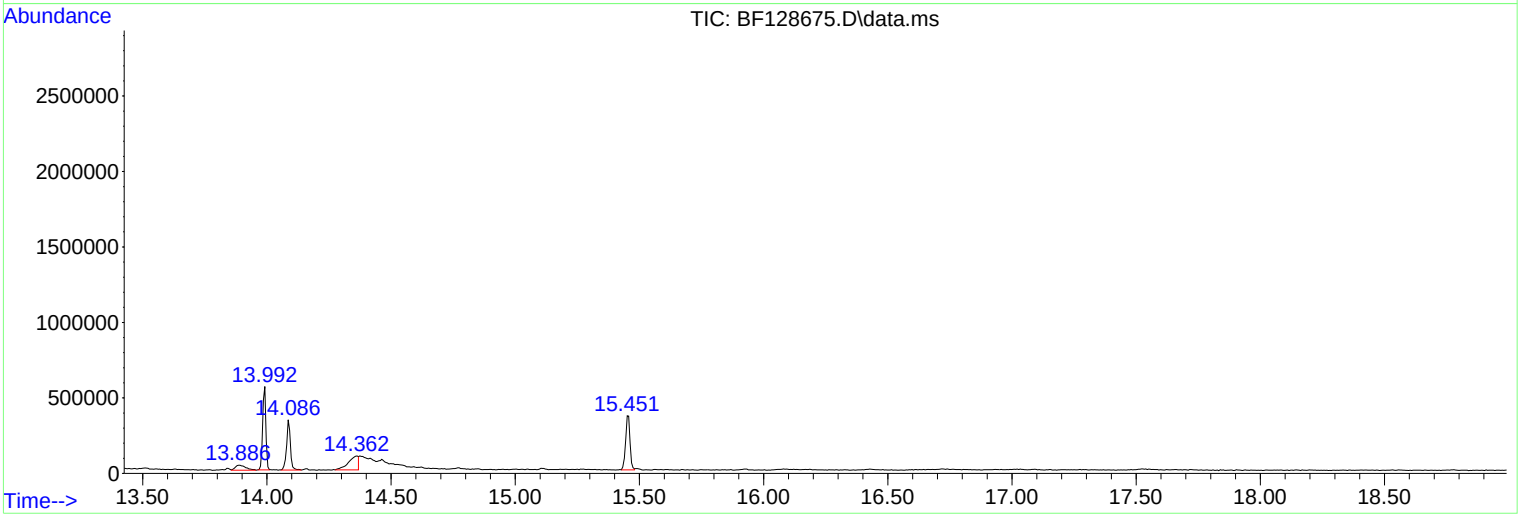
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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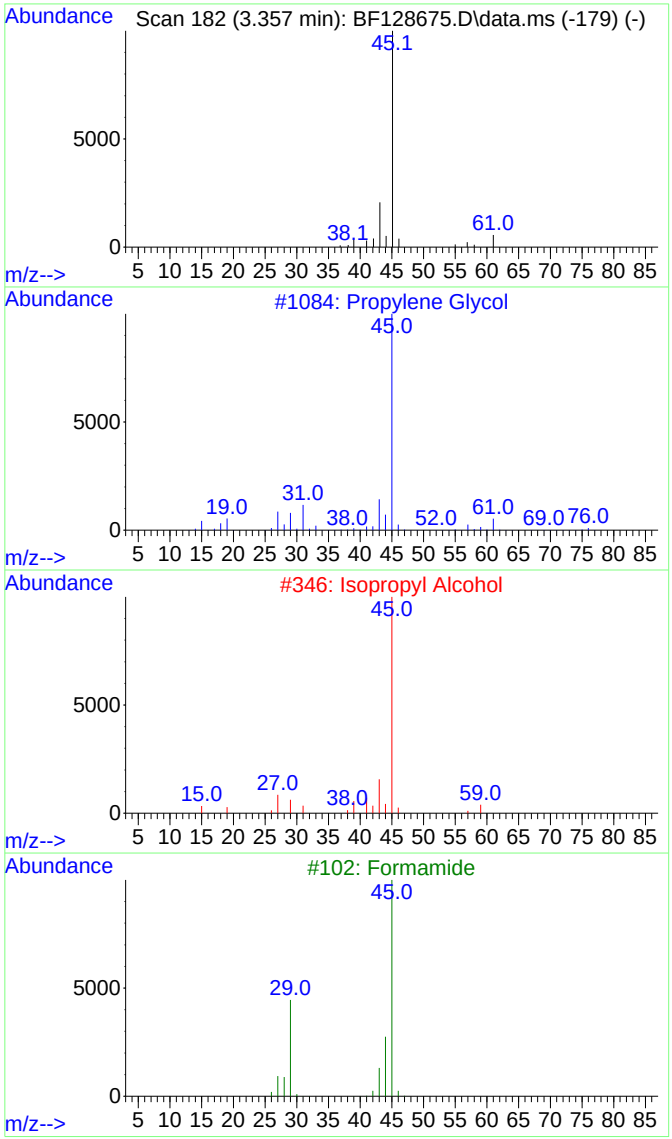
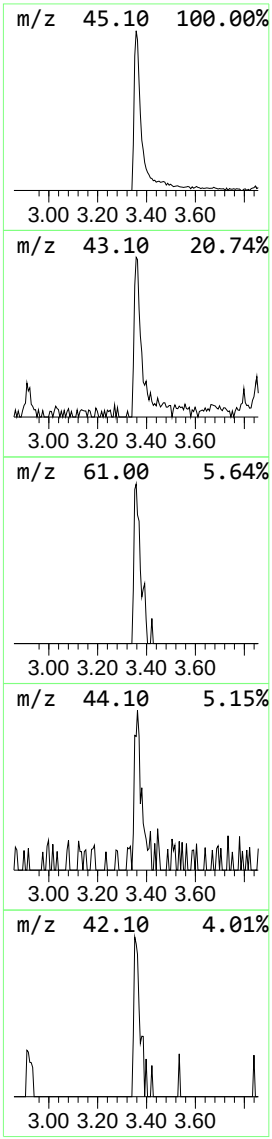
****

Peak Number 1 unknown3.357 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.357	2.28 ng	61591	1,4-Dichlorobenzene-d4	6.822

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propylene Glycol	76	C3H8O2	000057-55-6	9
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	Formamide	45	CH3NO	000075-12-7	5
4	Methyltartronic acid	134	C4H6O5	000595-98-2	4
5	2,3-Butanediol	90	C4H10O2	000513-85-9	4





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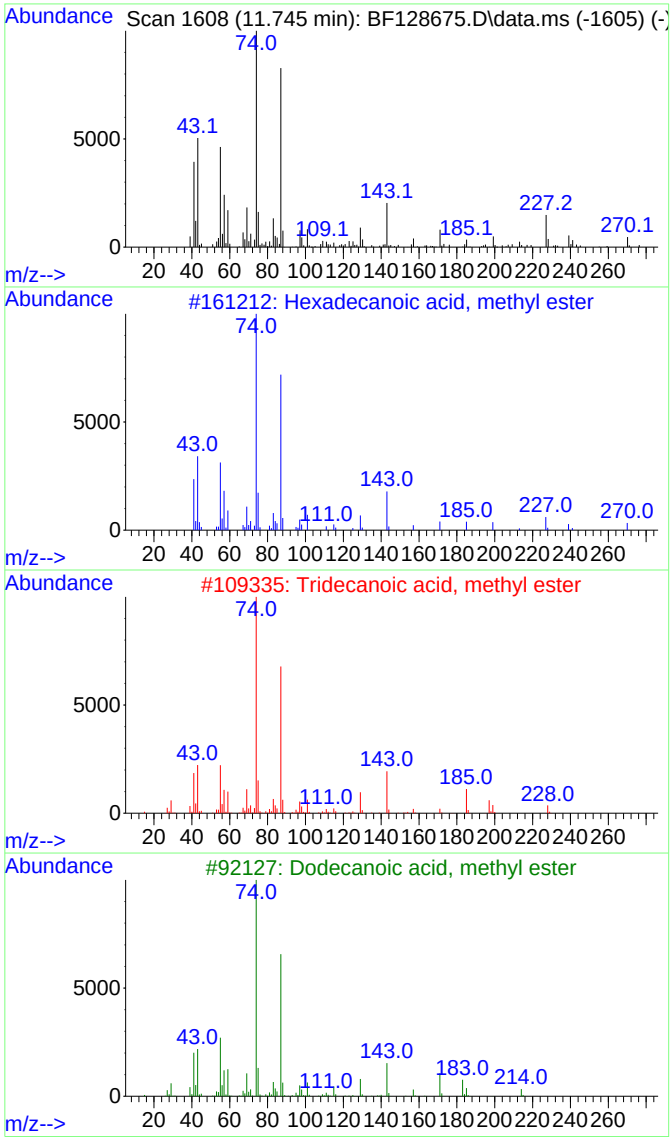
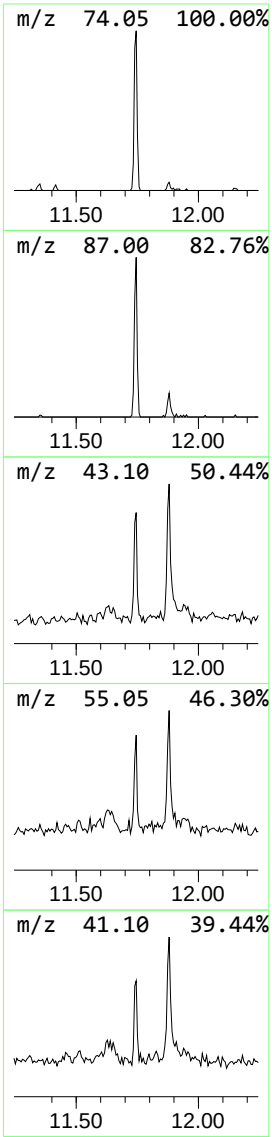
****
Peak Number 2 Hexadecanoic acid, methyl e... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.745	2.65 ng	101612	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	97
2	Tridecanoic acid, methyl ester	228	C14H28O2	001731-88-0	93
3	Dodecanoic acid, methyl ester	214	C13H26O2	000111-82-0	80
4	Tridecanoic acid, 12-methyl-, me...	242	C15H30O2	005129-58-8	80
5	Decanoic acid, methyl ester	186	C11H22O2	000110-42-9	72





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TIC Library : C:\Database\NIST20.L
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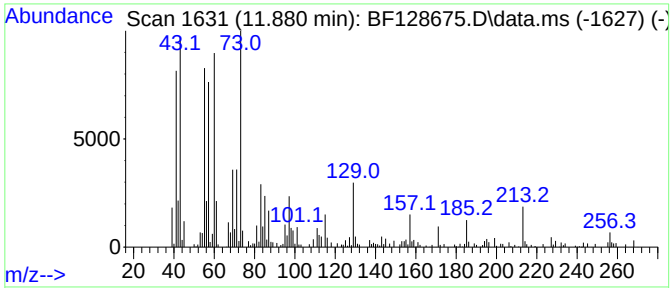
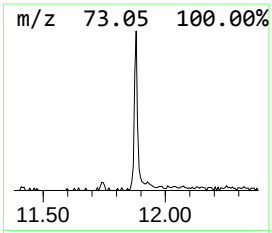
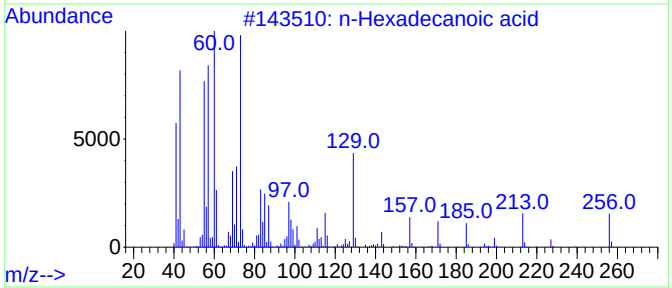
Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

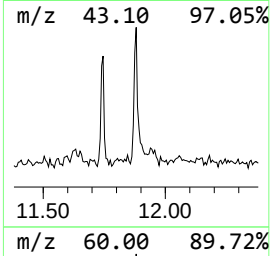
R.T.	EstConc	Area	Relative to ISTD	R.T.
11.880	4.42 ng	169171	Phenanthrene-d10	11.351

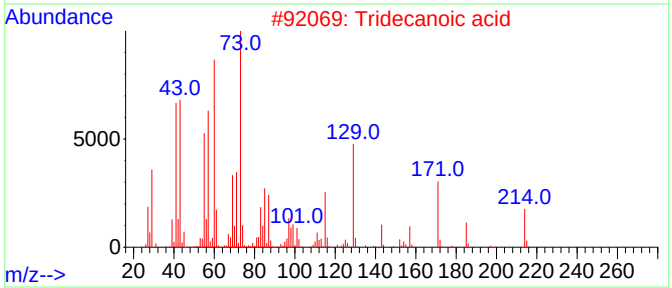
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	80
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5	Undecanoic acid	186	C11H22O2	000112-37-8	53

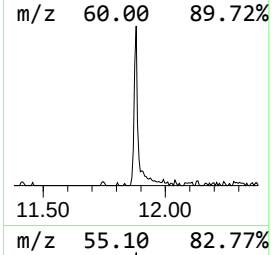


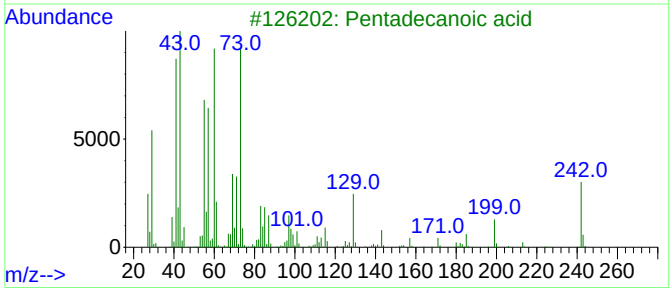


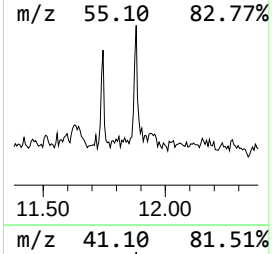


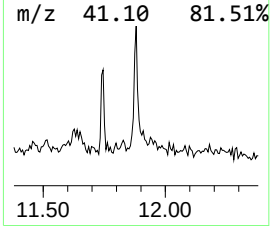












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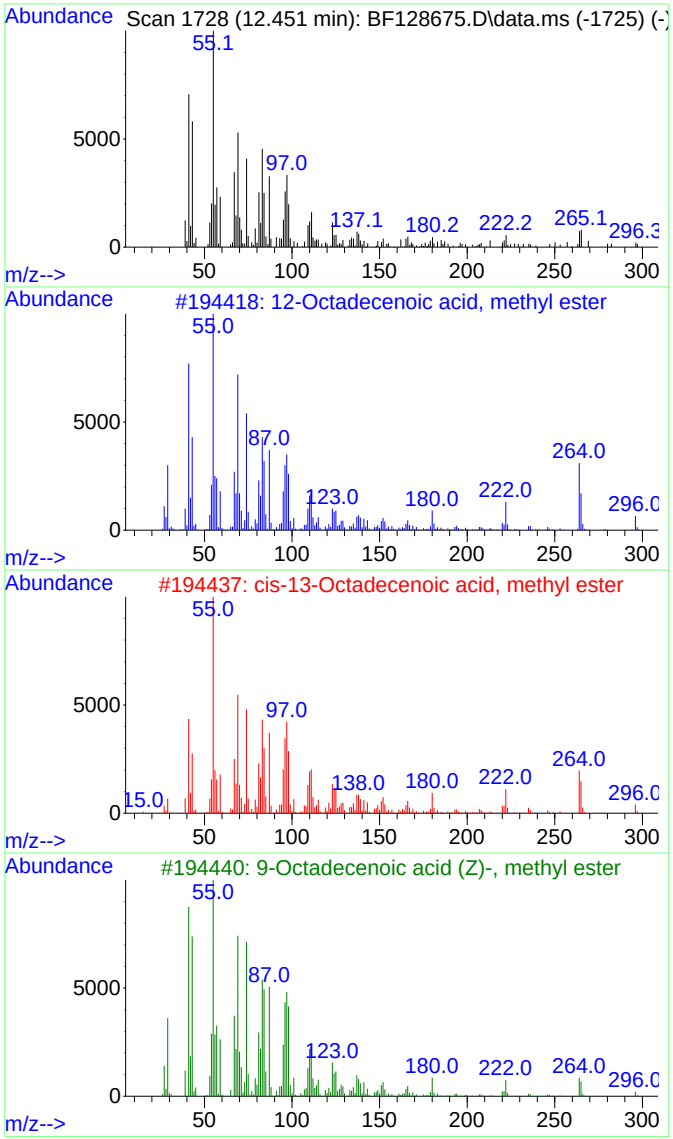
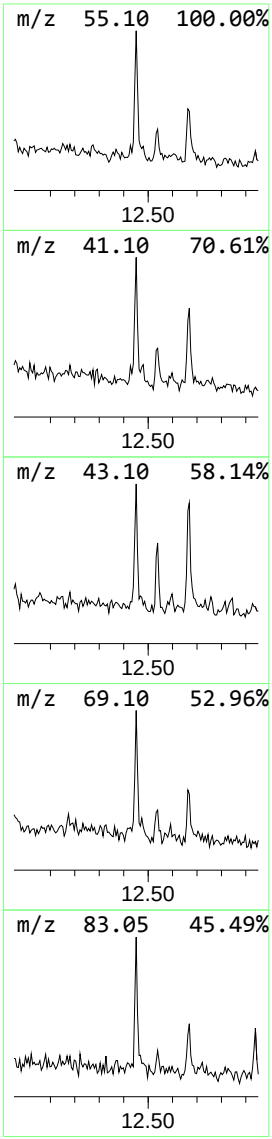
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 12-Octadecenoic acid, methy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.451	2.50 ng	95589	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
2	cis-13-Octadecenoic acid, methyl...	296	C19H36O2	1010333-58-3	99
3	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	99
4	10-Octadecenoic acid, methyl ester	296	C19H36O2	013481-95-3	99
5	11-Octadecenoic acid, methyl est...	296	C19H36O2	001937-63-9	98





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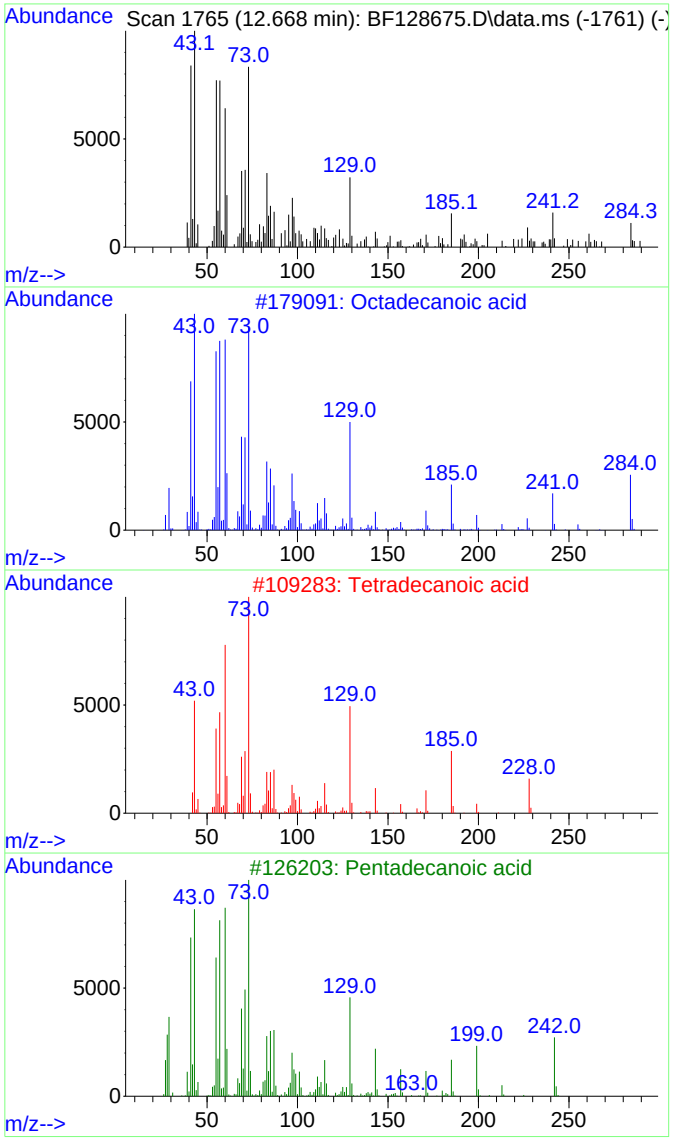
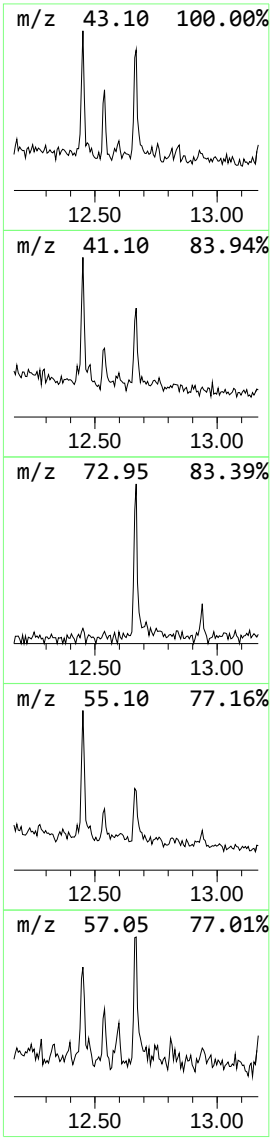
****

Peak Number 5 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.669	2.35 ng	89960	Phenanthrene-d10	11.351

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	86
4	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	83
5	n-Decanoic acid	172	C10H20O2	000334-48-5	55





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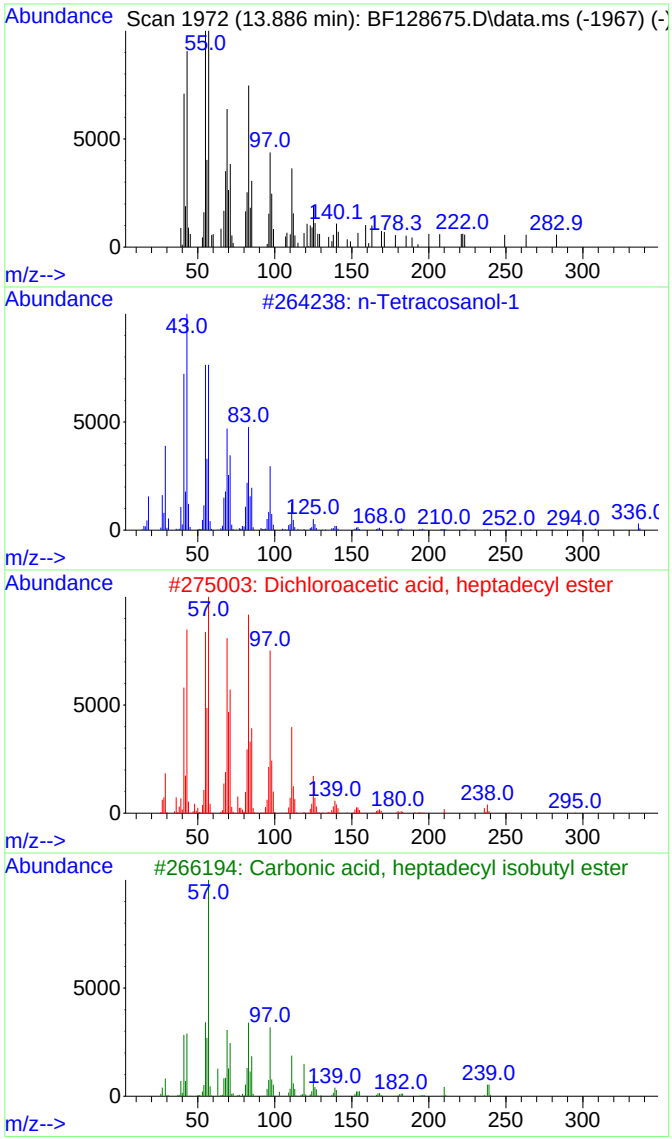
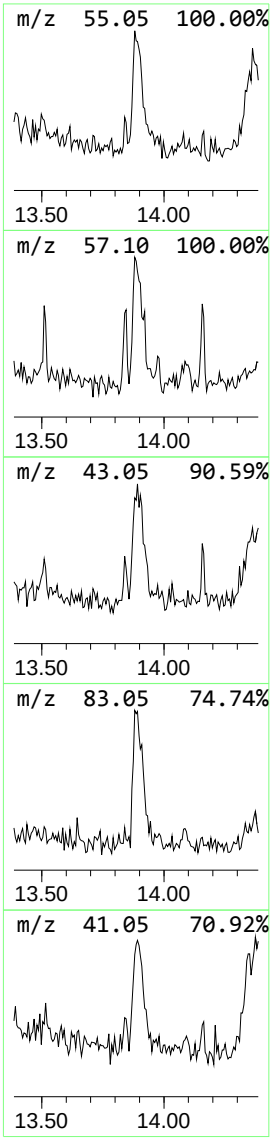
Peak Number 6 n-Tetracosanol-1 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.886	3.80 ng	94712	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	80
2	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	72
3	Carbonic acid, heptadecyl isobut...	356	C22H44O3	1000314-61-4	72
4	n-Heptadecanol-1	256	C17H36O	001454-85-9	64
5	Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	64





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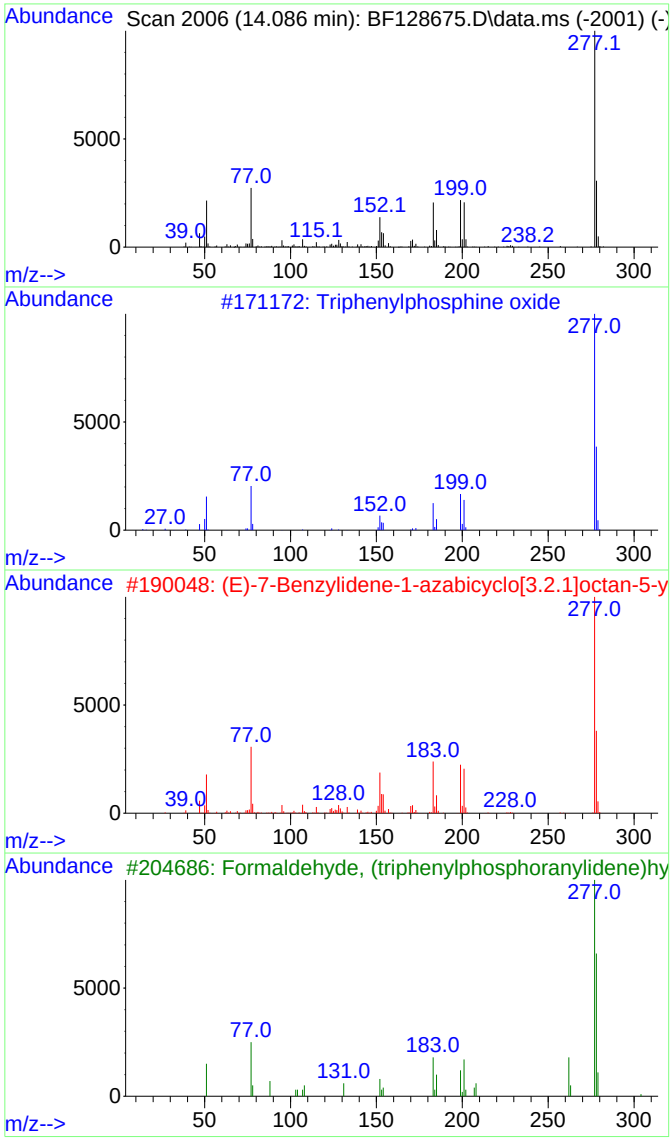
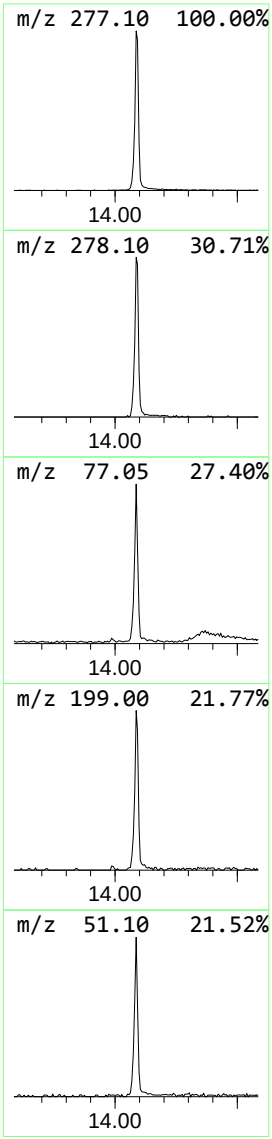
Peak Number 7 Triphenylphosphine oxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.086	13.96 ng	348069	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	97
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	93
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	64
4	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	38
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	37





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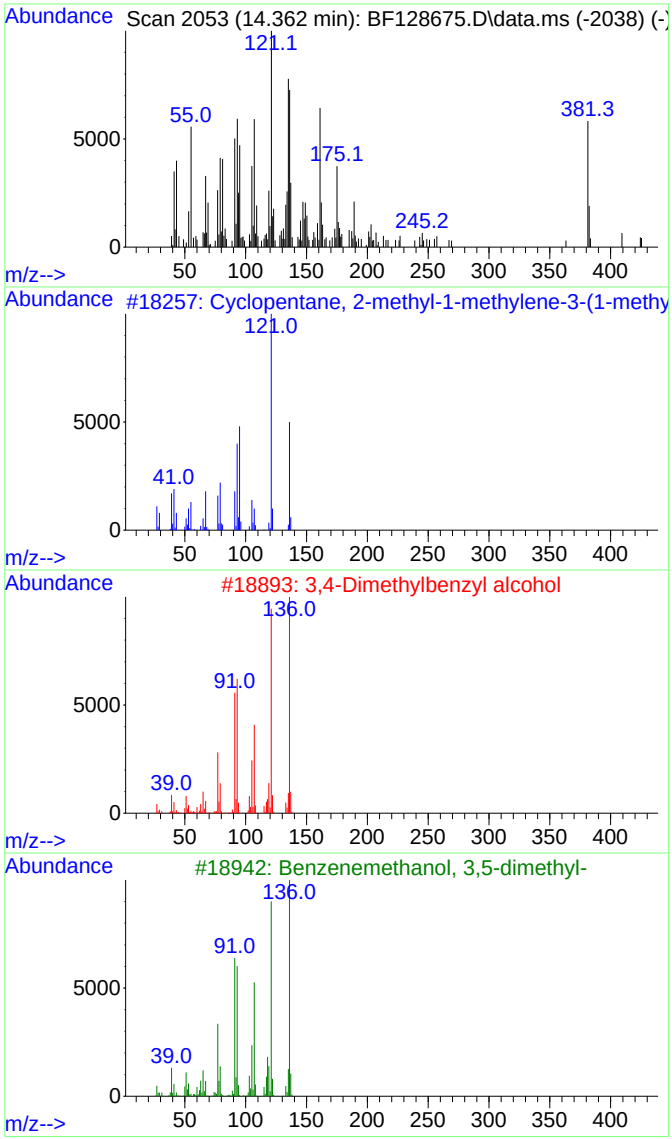
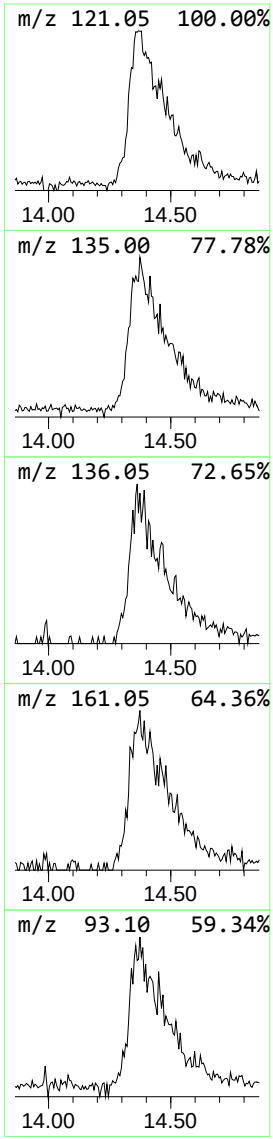
Peak Number 8 unknown14.363 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.363	10.38 ng	258861	Chrysene-d12	13.992

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentane, 2-methyl-1-methyle...	136	C10H16	056710-83-9	38
2	3,4-Dimethylbenzyl alcohol	136	C9H12O	006966-10-5	38
3	Benzenemethanol, 3,5-dimethyl-	136	C9H12O	027129-87-9	38
4	2,4,6-Octatriene, 3,4-dimethyl-	136	C10H16	057396-75-5	35
5	2,6,6-Trimethylcyclohexa-1,4-die...	150	C10H14O	162376-82-1	35





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF060322\
Data File : BF128675.D
Acq On : 03 Jun 2022 12:46
Operator : CG\JU
Sample : N3025-05
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
UST-BOT

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF060222.M
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
unknown3.357	3.357	2.3	ng	61591	1	6.822	540403	20.0
Hexadecanoic ac...	11.745	2.6	ng	101612	4	11.351	765529	20.0
n-Hexadecanoic ...	11.880	4.4	ng	169171	4	11.351	765529	20.0
12-Octadecenoic...	12.451	2.5	ng	95589	4	11.351	765529	20.0
Octadecanoic acid	12.669	2.4	ng	89960	4	11.351	765529	20.0
n-Tetracosanol-1	13.886	3.8	ng	94712	5	13.992	498608	20.0
Triphenylphosph...	14.086	14.0	ng	348069	5	13.992	498608	20.0
unknown14.363	14.363	10.4	ng	258861	5	13.992	498608	20.0