LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011223\
Data File : BF132048.D
Acq On : 12 Jan 2023 18:46
Operator : CG\JU
Sample : 01106-01
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument : BNA_F
ClientSampleId : MH-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-BF010923.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132048.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.975	486	491	504	rVB	611611	853888	34.38%	5.515%
2	5.393	558	562	580	rBV	2156097	1968784	79.27%	12.716%
3	6.416	732	736	739	rBV	2052119	1989187	80.09%	12.848%
4	6.769	792	796	800	rBV	572296	467404	18.82%	3.019%
5	7.345	889	894	897	rBV	1385003	1337146	53.84%	8.636%
6	8.057	1011	1015	1019	rBV	652919	585258	23.57%	3.780%
7	9.139	1194	1199	1202	rBV	2821155	2483577	100.00%	16.041%
8	9.816	1310	1314	1318	rBV	742592	679655	27.37%	4.390%
9	10.539	1433	1437	1440	rVB	54266	48226	1.94%	0.311%
10	10.616	1445	1450	1453	rBV	1475662	1366940	55.04%	8.829%
11	11.310	1564	1568	1571	rBV	796075	635173	25.57%	4.102%
12	12.716	1803	1807	1810	rBV	57737	45834	1.85%	0.296%
13	12.898	1834	1838	1841	rBV	2026927	1787343	71.97%	11.544%
14	13.421	1924	1927	1930	rVB2	34873	29642	1.19%	0.191%
15	13.792	1987	1990	2001	rBV	111606	212517	8.56%	1.373%
16	13.957	2014	2018	2022	rBV	466517	398191	16.03%	2.572%
17	14.704	2142	2145	2151	rBV2	109201	133599	5.38%	0.863%
18	14.792	2157	2160	2164	rVB	36583	31994	1.29%	0.207%
19	15.415	2261	2266	2272	rBV	351057	428318	17.25%	2.766%

Sum of corrected areas: 15482676

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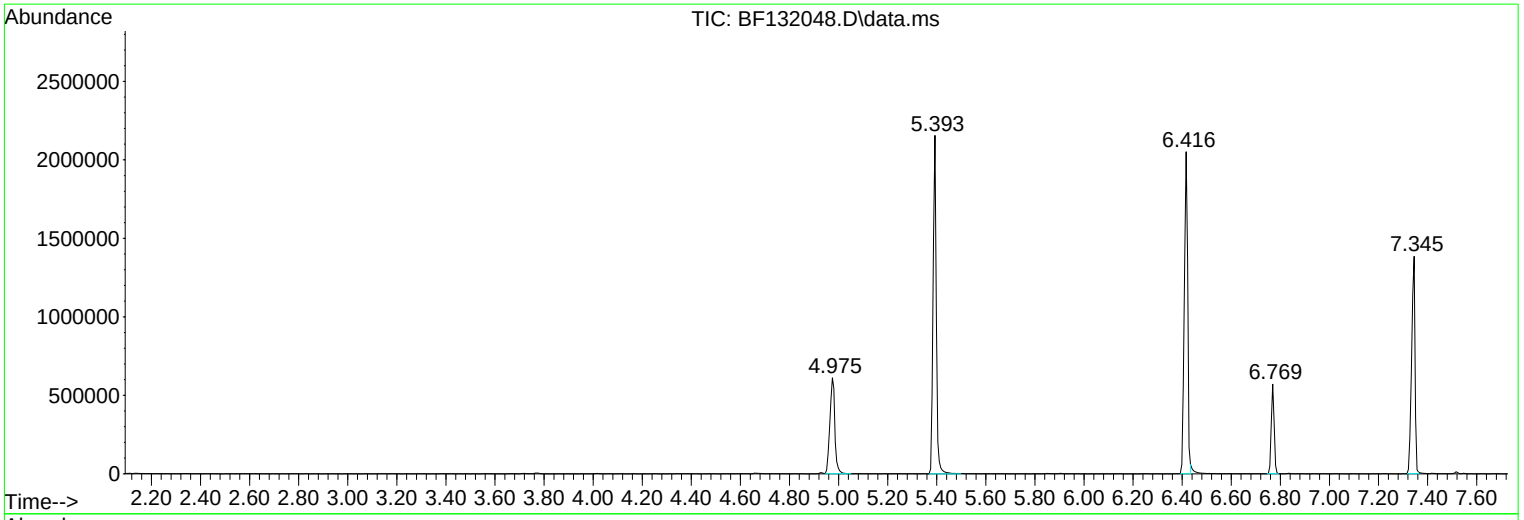
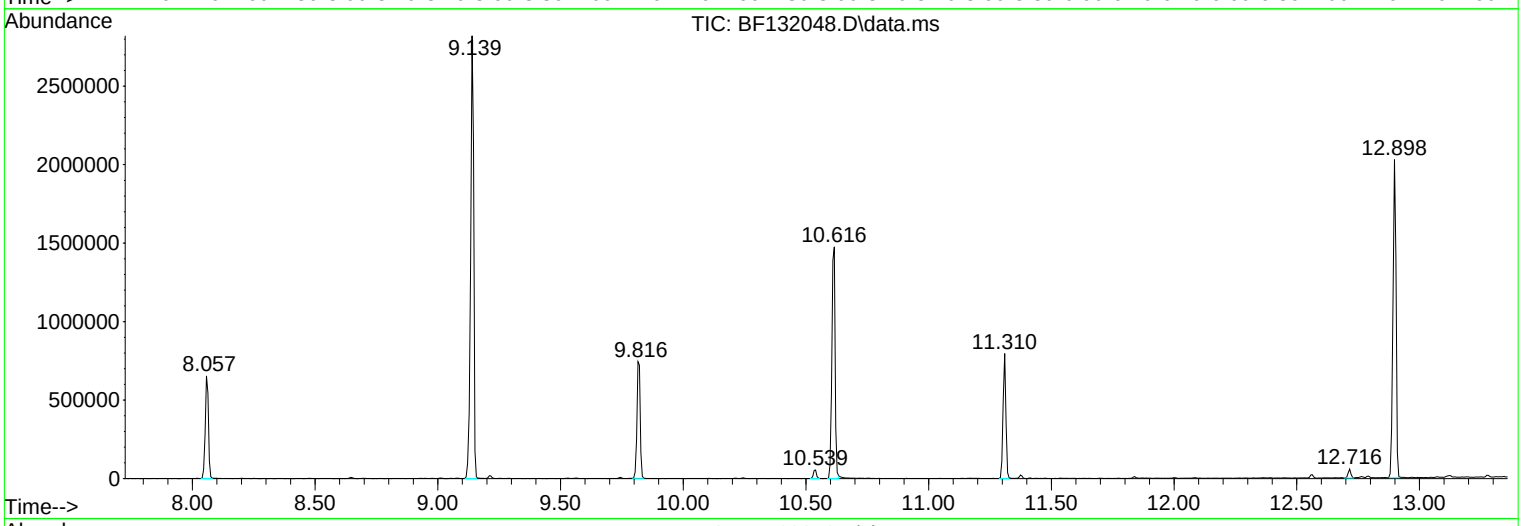
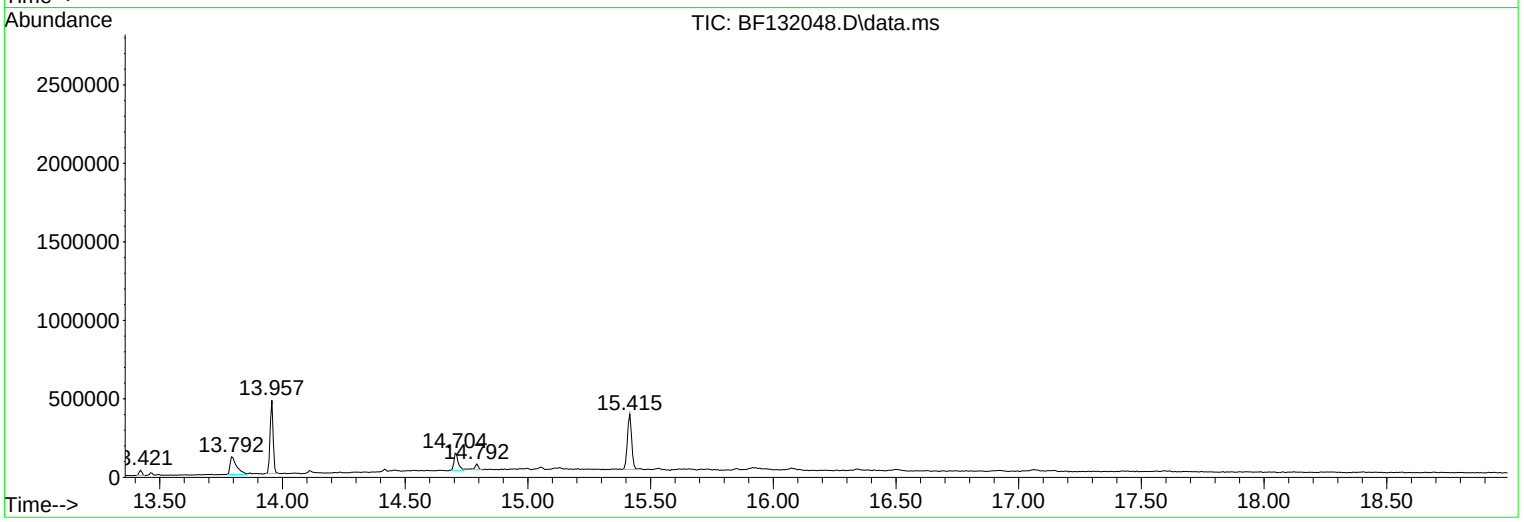
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF010923.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







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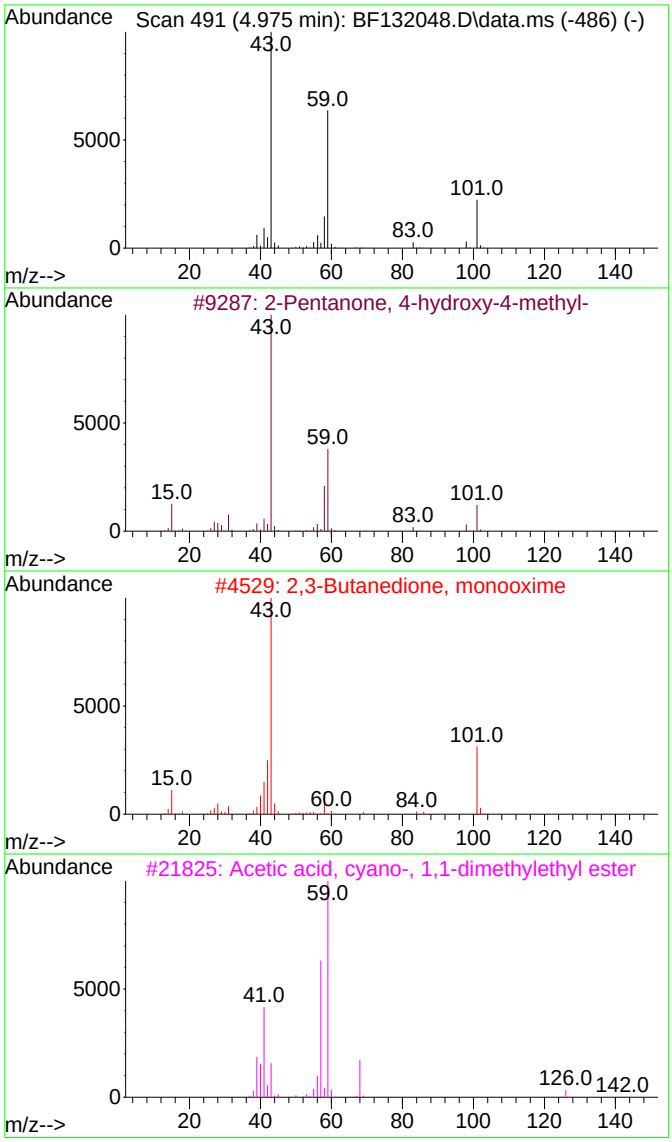
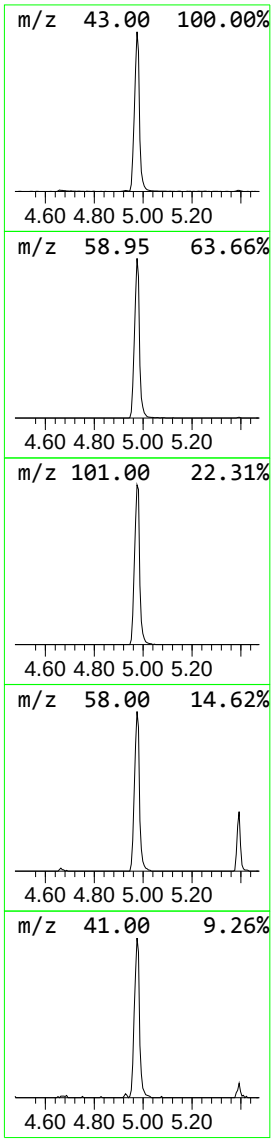
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.975	36.54 ng	853888	1,4-Dichlorobenzene-d4	6.769

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	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

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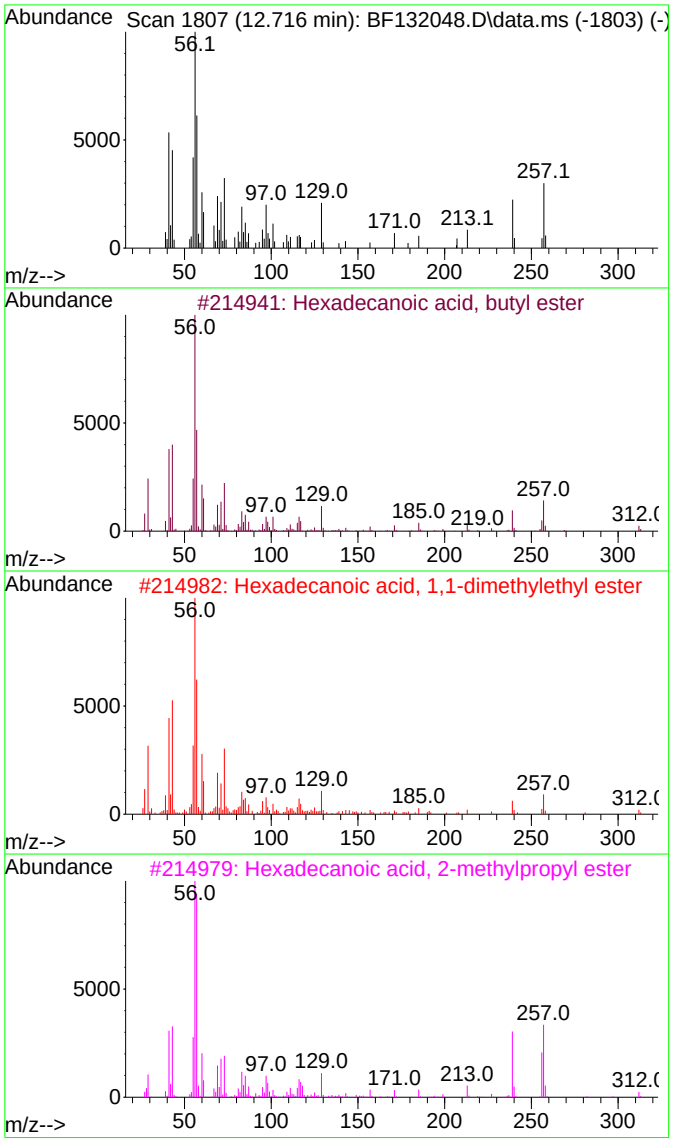
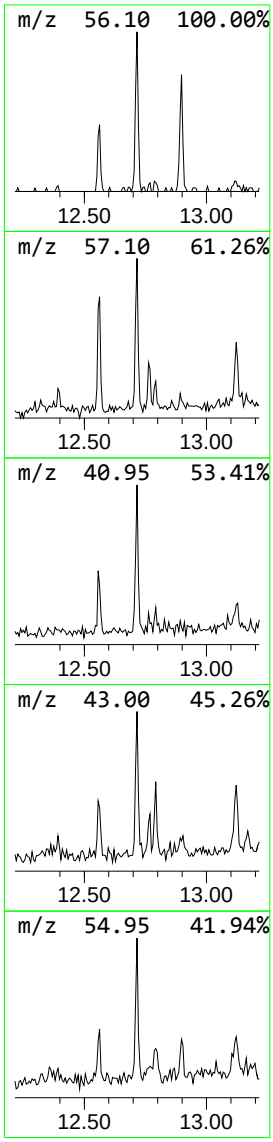
Peak Number 2 Hexadecanoic acid, butyl ester Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.716	2.30 ng	45834	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	64
2	Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	58
3	Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	43
4	2-Methyl-1-tetradecene	210	C15H30	052254-38-3	27
5	1,3-Cyclopentanedione, 4-butyl-	154	C9H14O2	054244-72-3	25





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Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
MH-3

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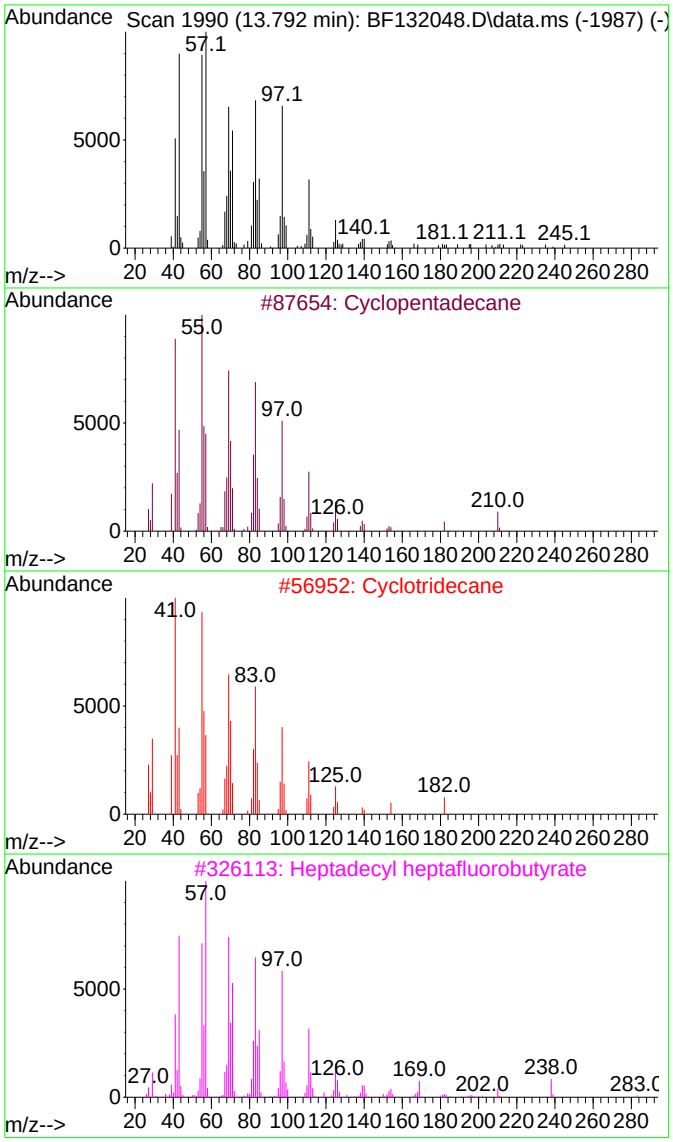
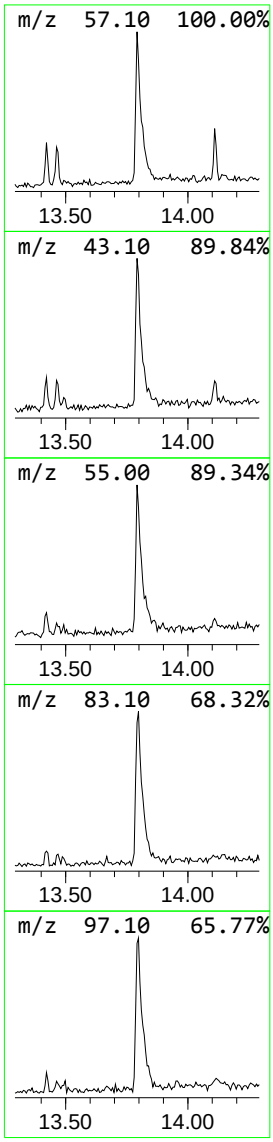
Peak Number 3 Cyclopentadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.792	10.67 ng	212517	Chrysene-d12	13.957

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Cyclopentadecane	210	C15H30	000295-48-7	97
2	Cyclotridecane	182	C13H26	000295-02-3	97
3	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
4	1-Heptacosanol	396	C27H56O	002004-39-9	91
5	Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	91





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Instrument :
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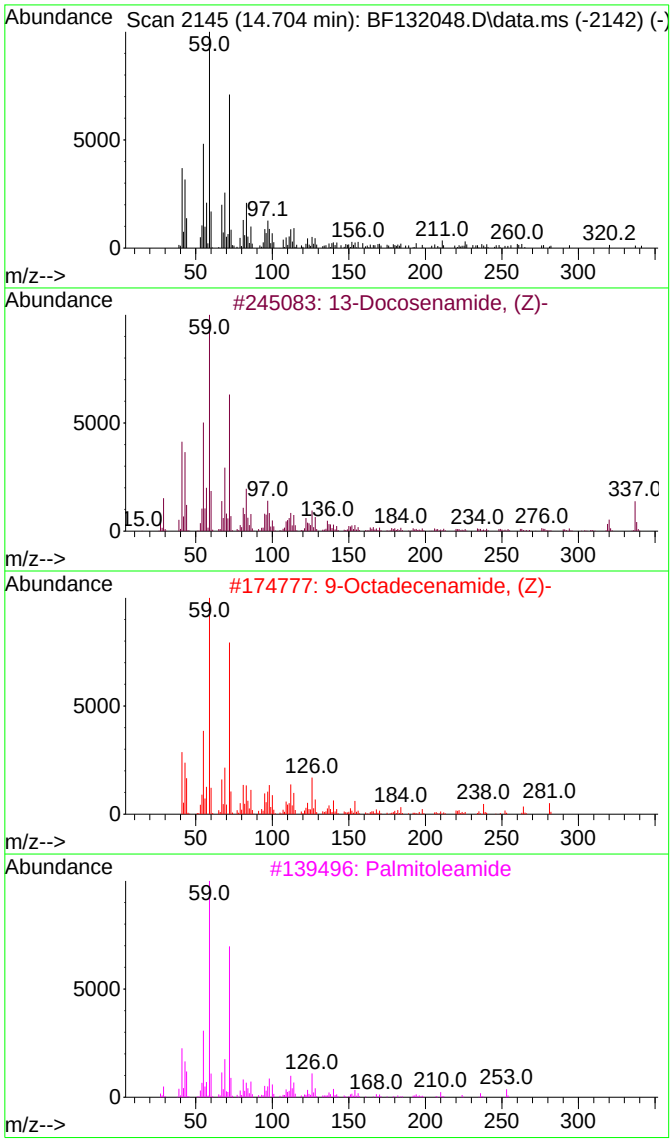
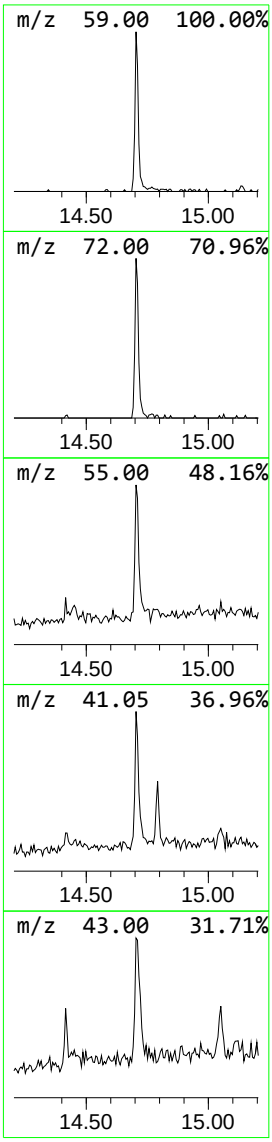
Peak Number 4 13-Docosenamide, (Z)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.704	6.24 ng	133599	Perylene-d12	15.416

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	91
2	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	68
3	Palmitoleamide	253	C16H31NO	106010-22-4	53
4	Tetradecanamide	227	C14H29NO	000638-58-4	49
5	Dodecanamide	199	C12H25NO	001120-16-7	43





Tentatively Identified Compound (LSC) summary

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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-...	4.975	36.5	ng	853888	1	6.769	467404	20.0
Hexadecanoic ac...	12.716	2.3	ng	45834	5	13.957	398191	20.0
Cyclopentadecane	13.792	10.7	ng	212517	5	13.957	398191	20.0
13-Docosenamide...	14.704	6.2	ng	133599	6	15.416	428318	20.0