LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
Data File : BF131743.D
Acq On : 21 Dec 2022 13:26
Operator : CG\JU
Sample : N6100-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-303-20221215

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-BF122022.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF131743.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.116	3	5	11	rVB	1689391	1690766	46.66%	9.159%
2	5.063	502	506	515	rVB	248807	253614	7.00%	1.374%
3	5.475	571	576	579	rBV	1081791	1045265	28.85%	5.663%
4	6.487	744	748	751	rBV	845519	675710	18.65%	3.661%
5	6.863	808	812	815	rBV	634686	505146	13.94%	2.737%
6	7.434	903	909	912	rBV	1797152	1915512	52.86%	10.377%
7	8.151	1027	1031	1035	rBV	746275	641304	17.70%	3.474%
8	9.234	1209	1215	1218	rBV	3477776	3623442	100.00%	19.629%
9	9.916	1326	1331	1334	rBV	933322	759694	20.97%	4.115%
10	10.710	1461	1466	1469	rBV	2458668	2156148	59.51%	11.681%
11	11.410	1581	1585	1588	rBV	949591	819281	22.61%	4.438%
12	11.475	1592	1596	1600	rVB	123463	101838	2.81%	0.552%
13	12.204	1712	1720	1741	rVB4	27360	112604	3.11%	0.610%
14	13.004	1851	1856	1859	rBV	2707886	2382455	65.75%	12.906%
15	13.521	1932	1944	1954	rBV3	46705	121907	3.36%	0.660%
16	14.057	2031	2035	2039	rBV	610361	534241	14.74%	2.894%
17	14.151	2047	2051	2058	rBV	204007	223842	6.18%	1.213%
18	14.286	2064	2074	2085	rVB2	57201	143459	3.96%	0.777%
19	14.915	2175	2181	2189	rVB	48542	93233	2.57%	0.505%
20	15.551	2284	2289	2293	rBV	354622	459728	12.69%	2.490%
21	16.021	2363	2369	2382	rBV	30848	138510	3.82%	0.750%
22	16.392	2426	2432	2440	rBV3	23204	61658	1.70%	0.334%

Sum of corrected areas: 18459357

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ClientSampleId :
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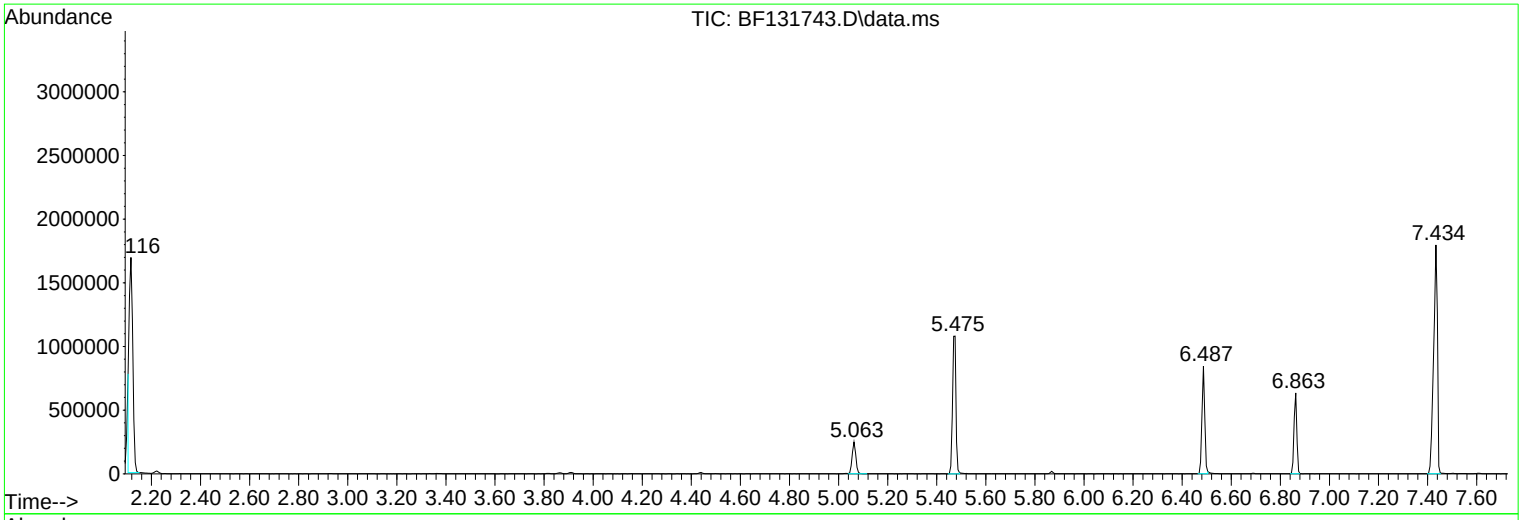
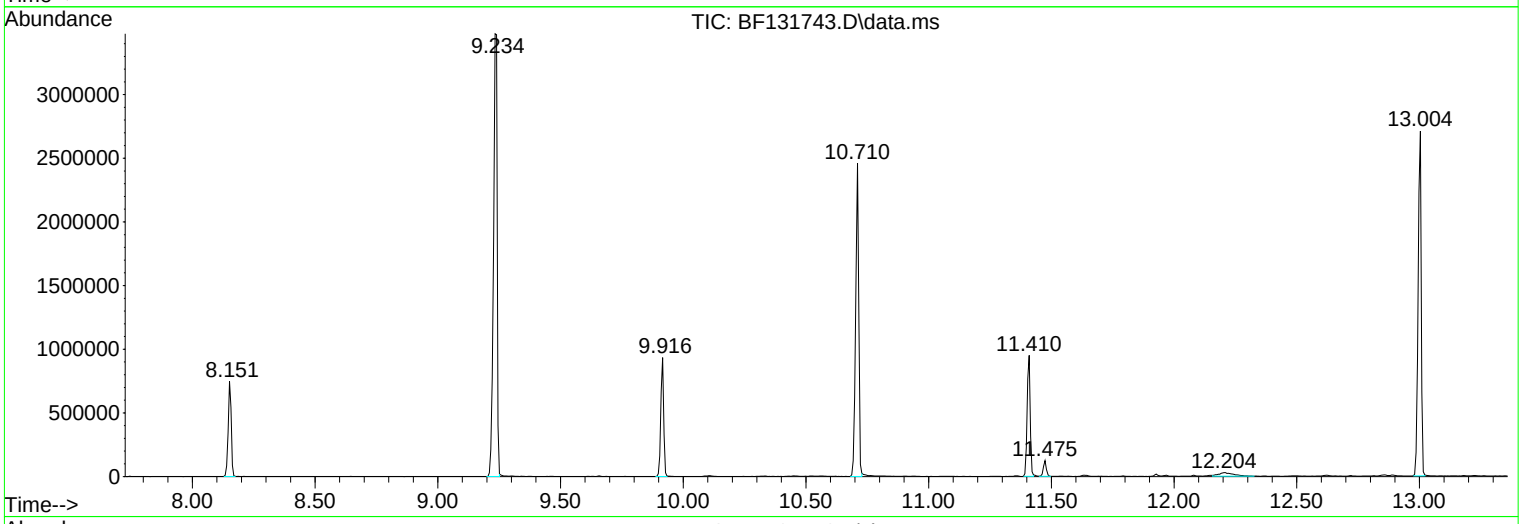
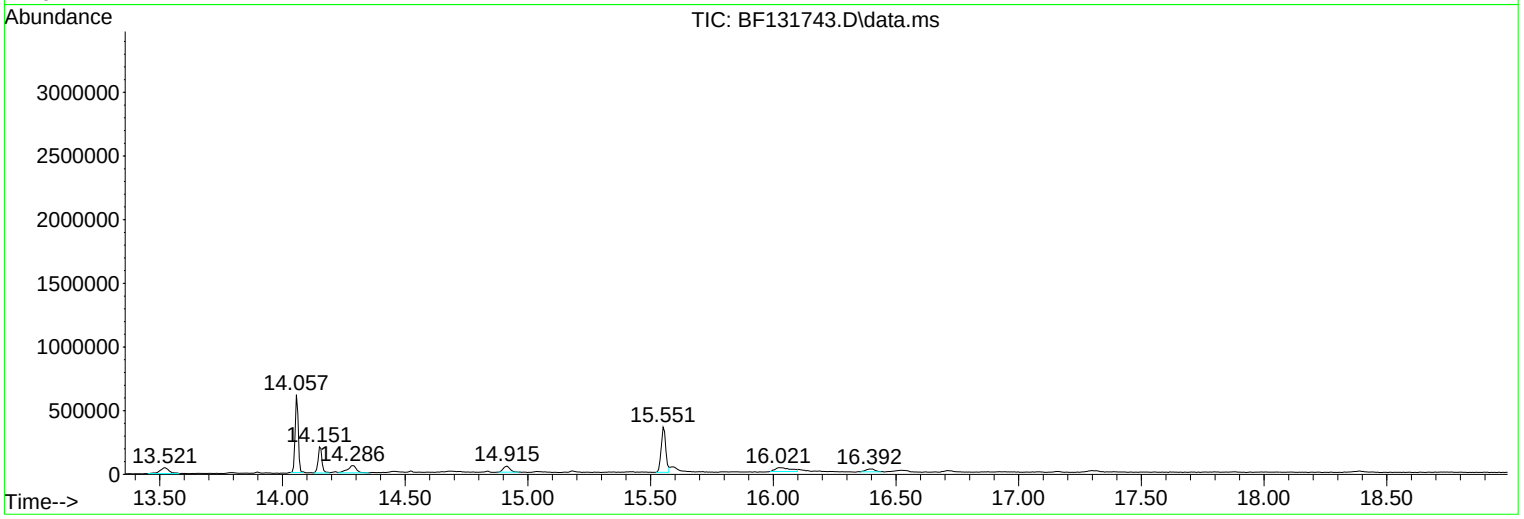
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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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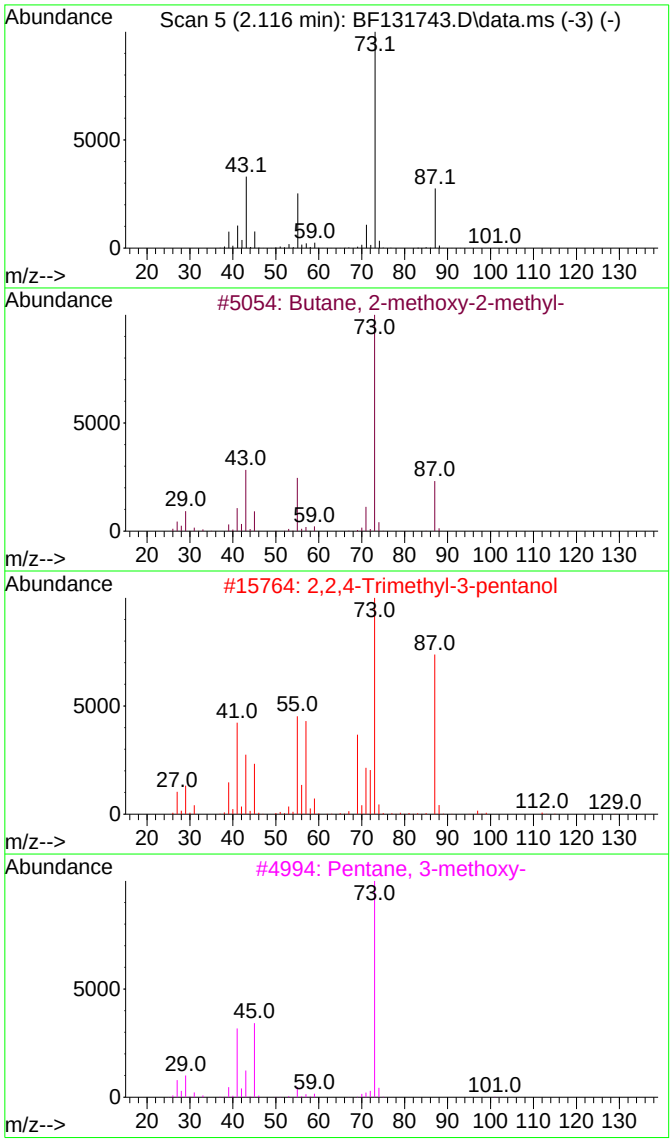
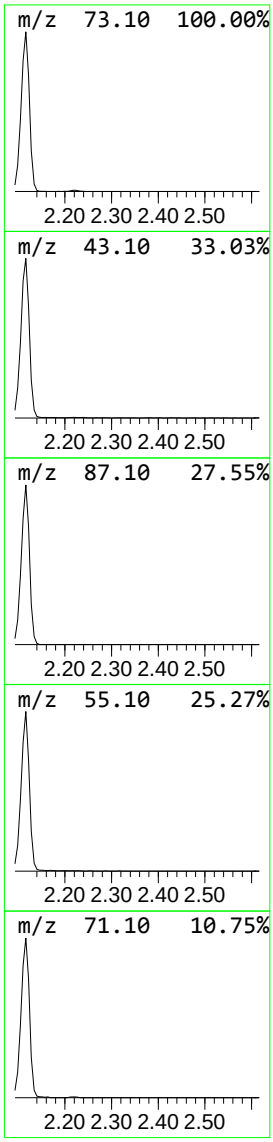
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.116	66.94 ng	1690770	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	39
3	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4	Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
5	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9





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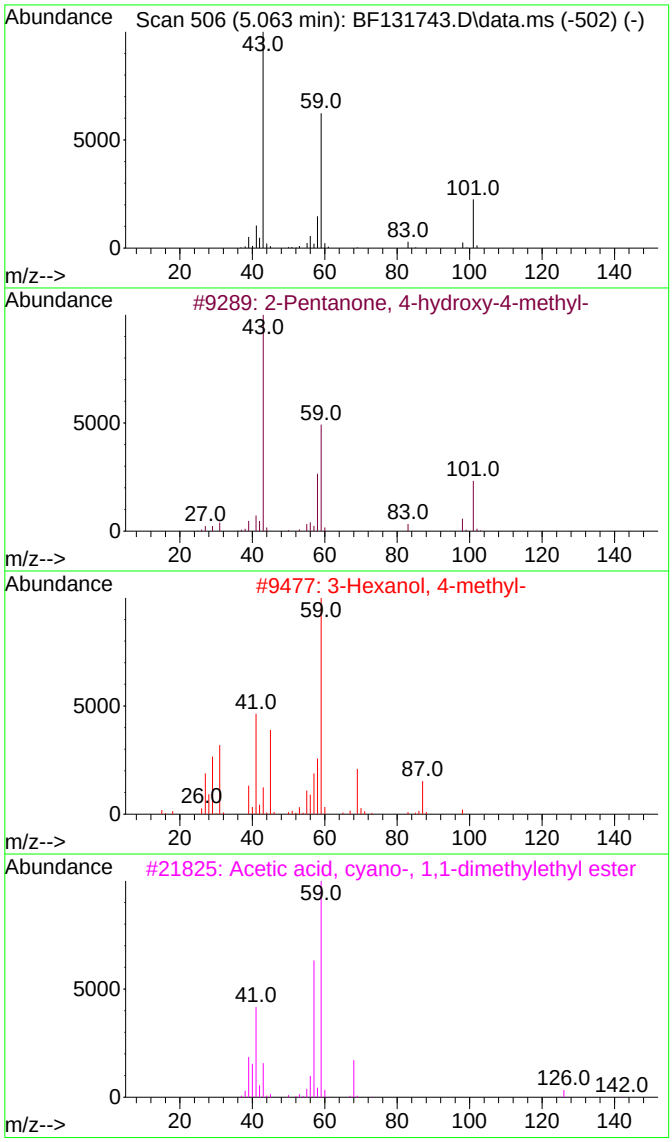
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

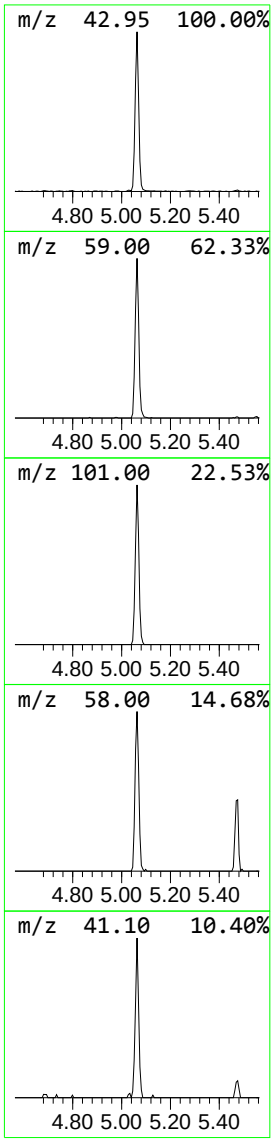
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.063	10.04 ng	253614	1,4-Dichlorobenzene-d4	6.863

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
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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ALS Vial : 6 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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TIC Integration Parameters: LSCINT.P

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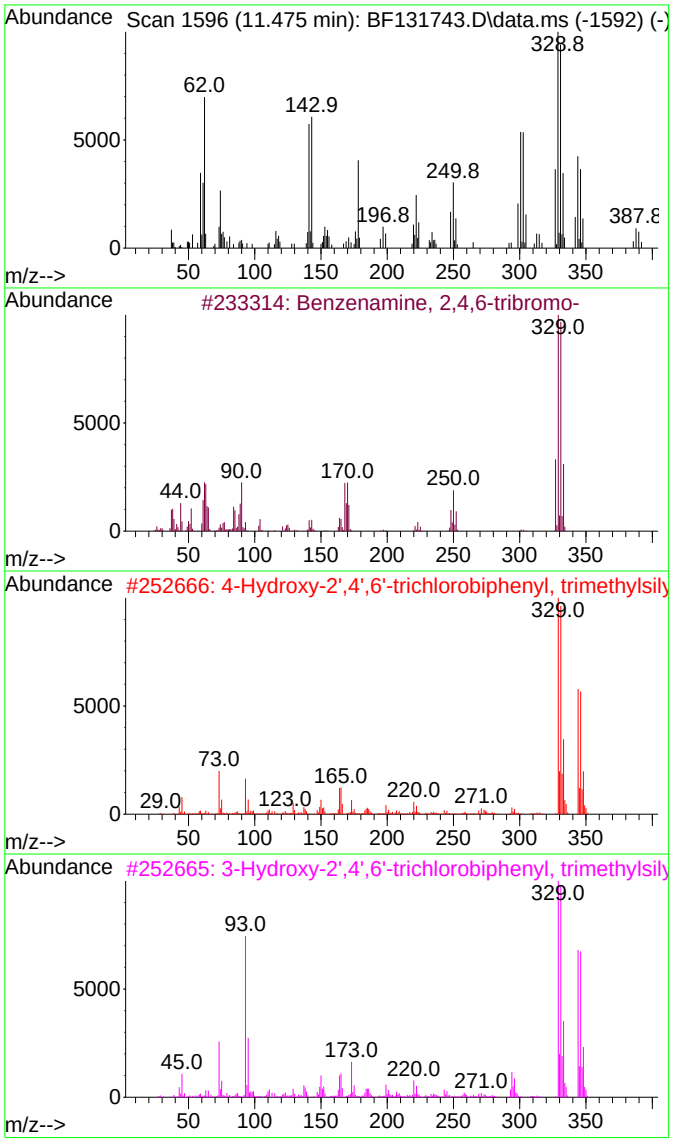
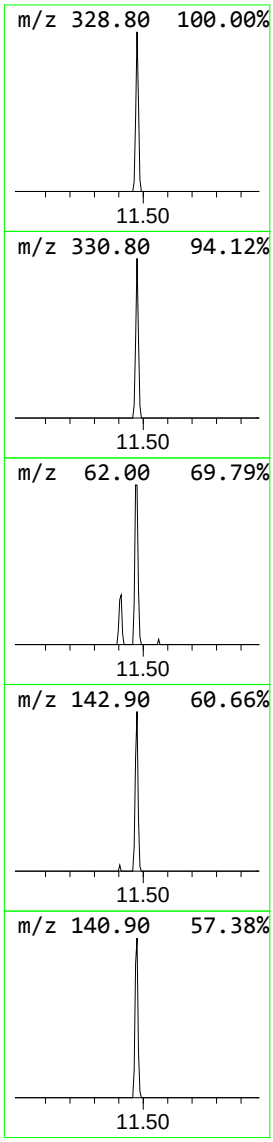
Peak Number 3 Benzenamine, 2,4,6-tribromo- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.475	2.49 ng	101838	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzenamine, 2,4,6-tribromo-	327	C6H4Br3N	000147-82-0	55
2	4-Hydroxy-2',4',6'-trichlorobiph...	344	C15H15Cl3OSi	1000447-71-9	46
3	3-Hydroxy-2',4',6'-trichlorobiph...	344	C15H15Cl3OSi	1000447-69-8	46
4	4-Hydroxy-2,2',5'-trichlorobiphe...	344	C15H15Cl3OSi	1000447-70-4	35
5	Trimethylsilyl 3-chloro-5-methox...	346	C14H23ClO4Si2	1000385-75-2	25





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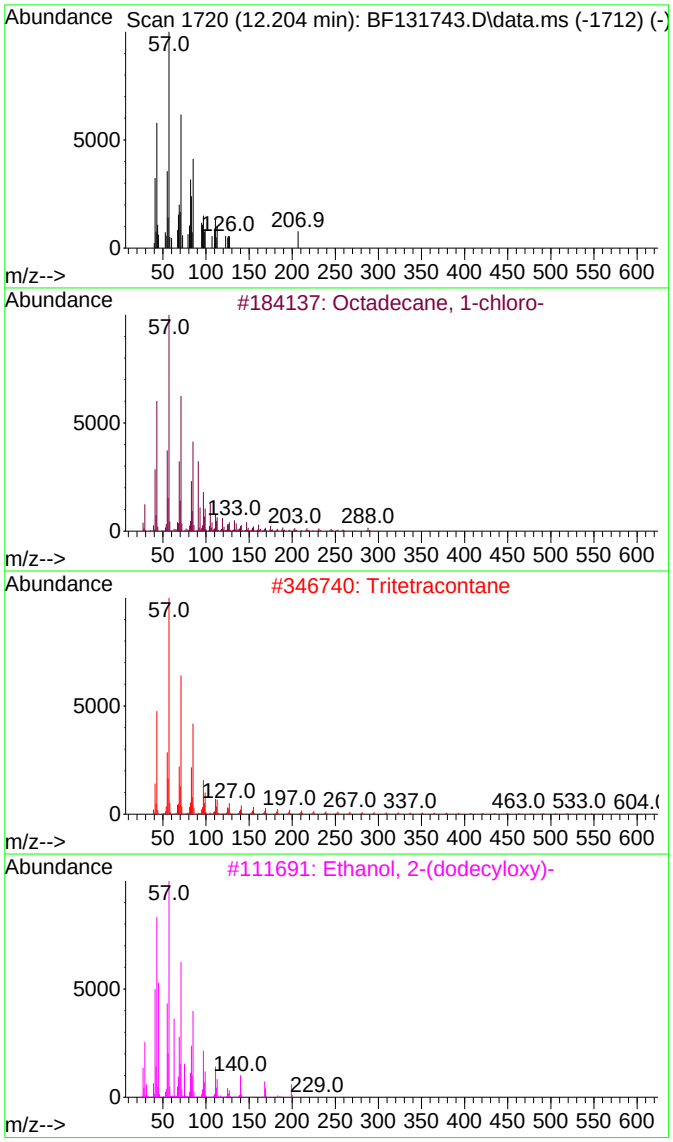
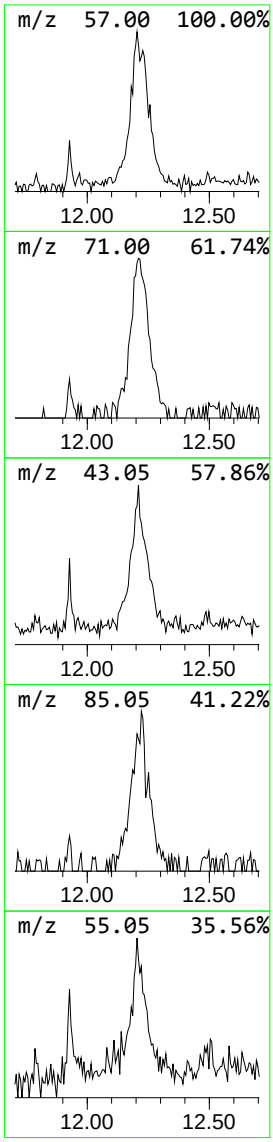
****

Peak Number 4 Octadecane, 1-chloro- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.204	2.75 ng	112604	Phenanthrene-d10	11.410

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane, 1-chloro-	288	C18H37Cl	003386-33-2	64
2	Tritetracontane	605	C43H88	007098-21-7	64
3	Ethanol, 2-(dodecyloxy)-	230	C14H30O2	004536-30-5	64
4	Carbonic acid, dodecyl vinyl ester	256	C15H28O3	1000382-54-8	64
5	Tetratetracontane	619	C44H90	007098-22-8	58





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TIC Library : C:\Database\NIST20.L
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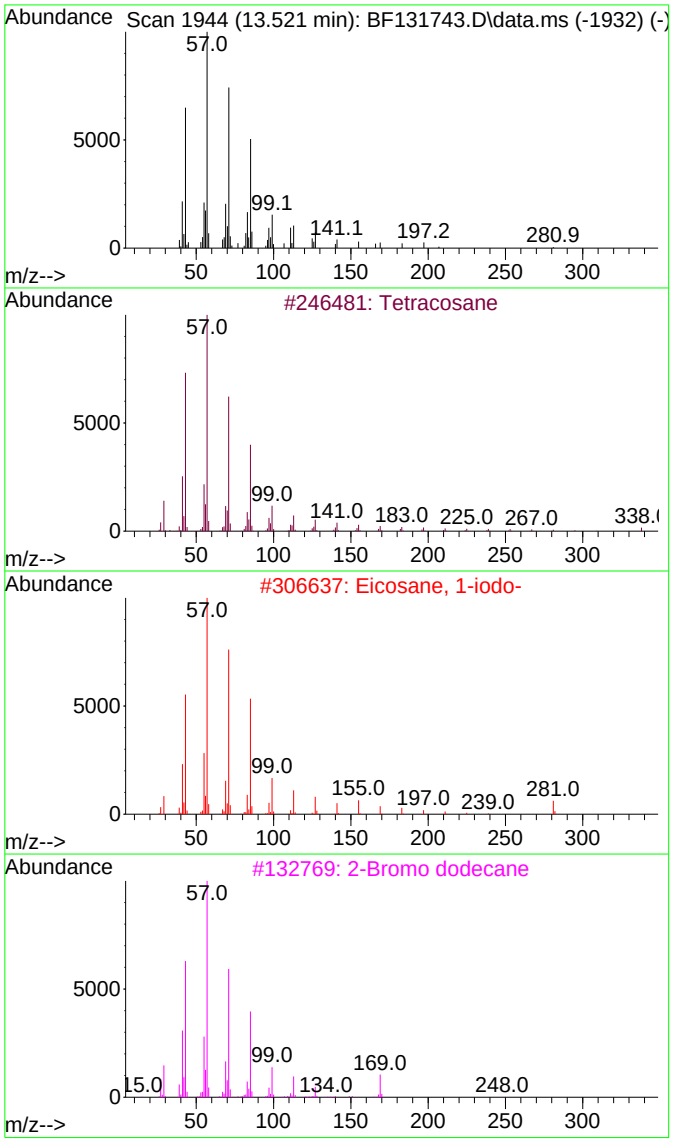
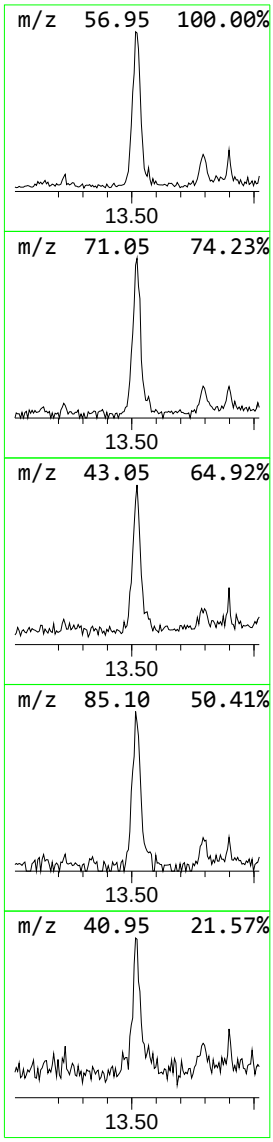
Peak Number 5 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.522	4.56 ng	121907	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	87
2	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	86
3	2-Bromo dodecane	248	C12H25Br	013187-99-0	86
4	Docosane	310	C22H46	000629-97-0	86
5	Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	86





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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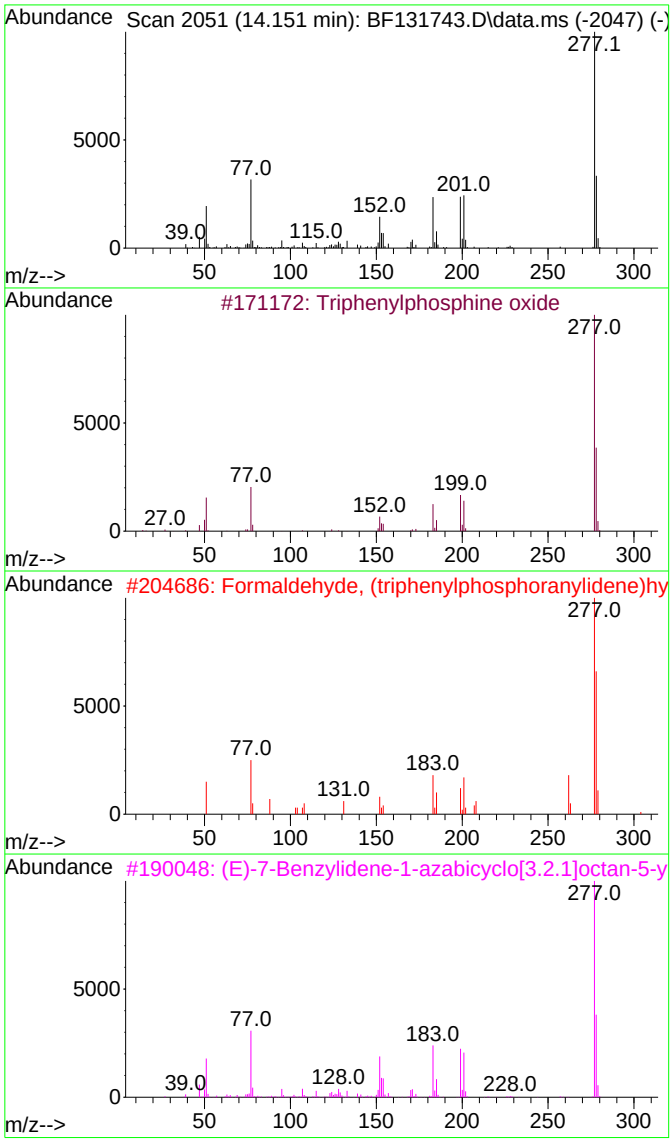
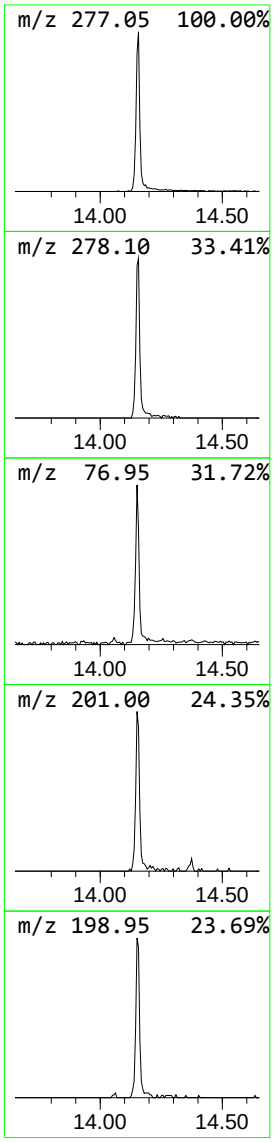
Peak Number 6 Triphenylphosphine oxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.151	8.38 ng	223842	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	86
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	49
4	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	38
5	cyclopenta[d][1,3]thiazine-2,4-d...	277	C13H11NS3	1000397-11-2	25





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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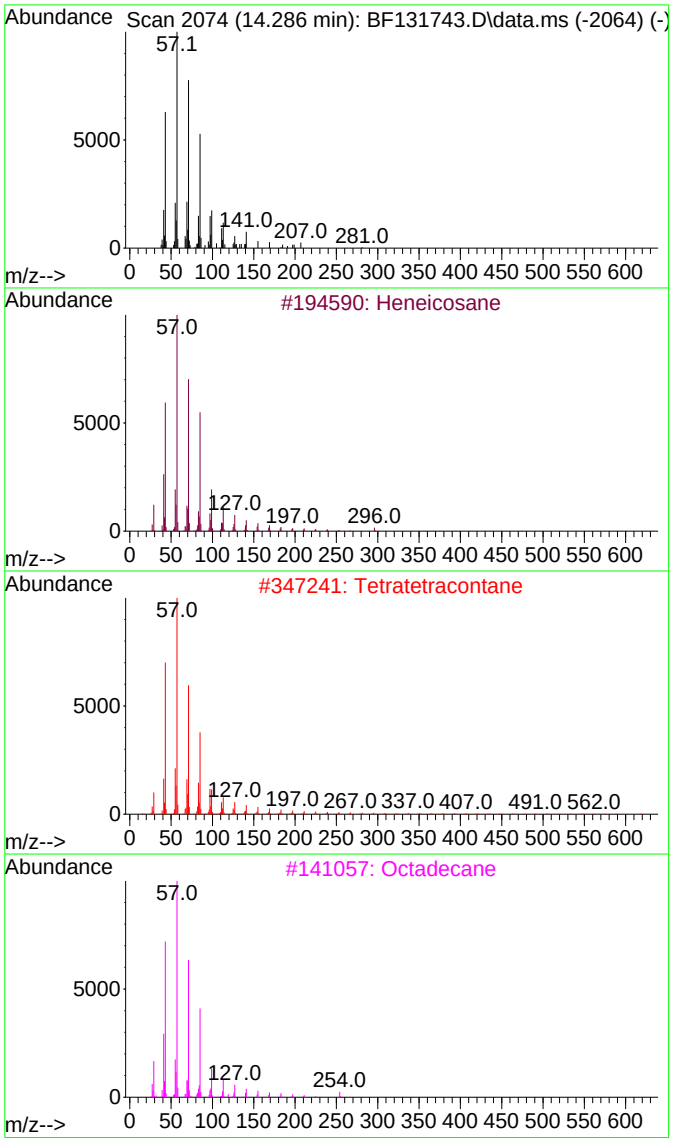
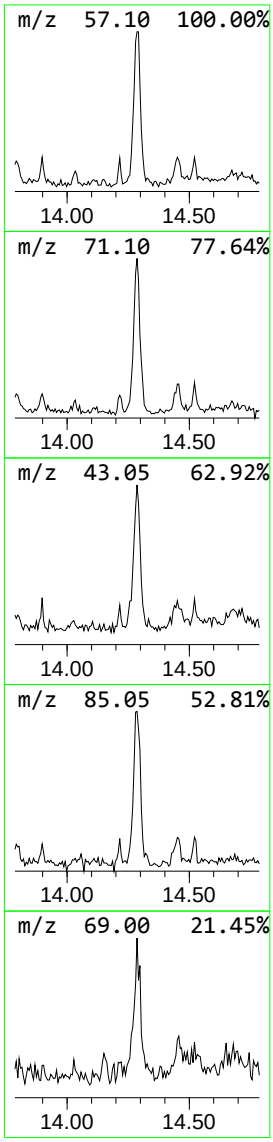
Peak Number 7 Heneicosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.286	5.37 ng	143459	Chrysene-d12	14.057

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heneicosane	296	C21H44	000629-94-7	87
2	Tetratetracontane	619	C44H90	007098-22-8	83
3	Octadecane	254	C18H38	000593-45-3	83
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5	Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	72





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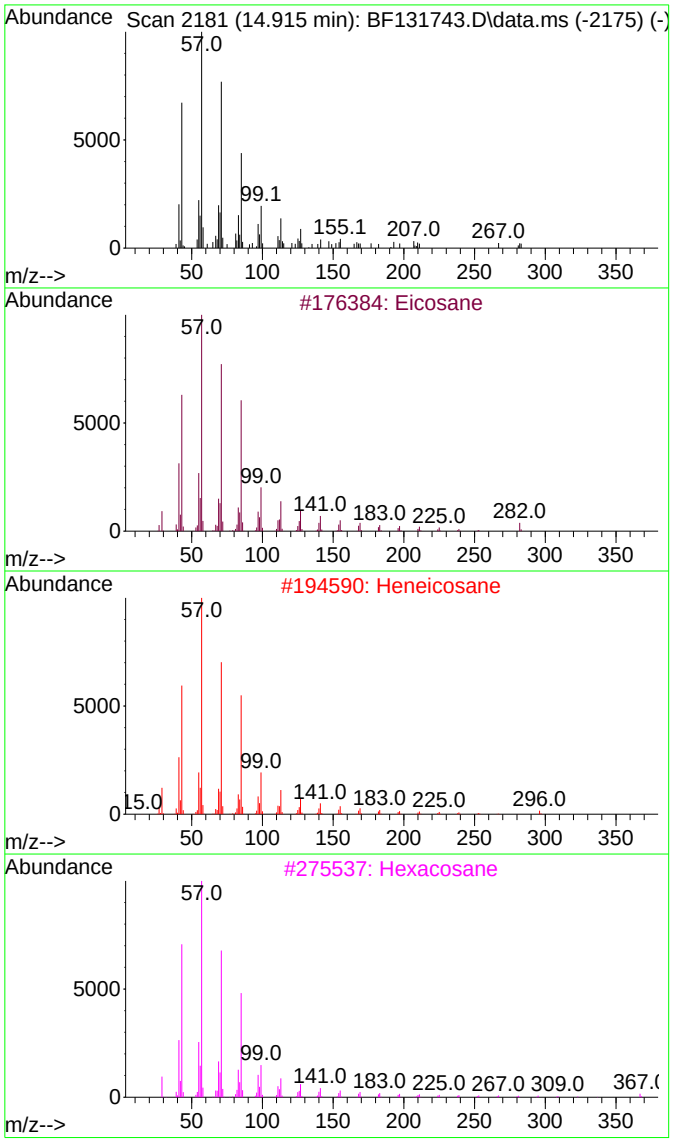
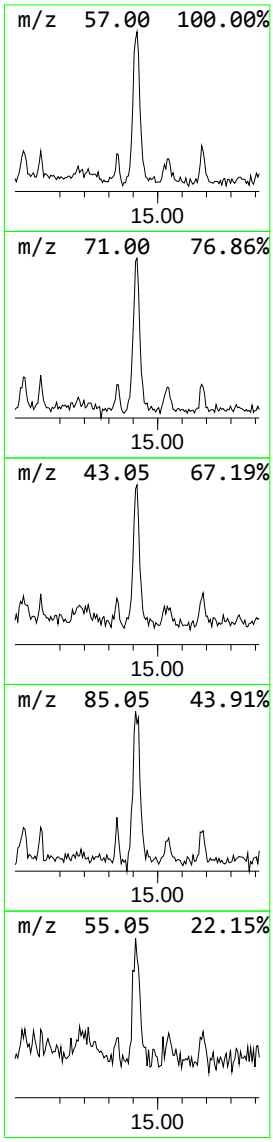
Peak Number 8 Eicosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.916	4.06 ng	93233	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Hentriacontane	437	C31H64	000630-04-6	91
5	Heptadecane	240	C17H36	000629-78-7	91





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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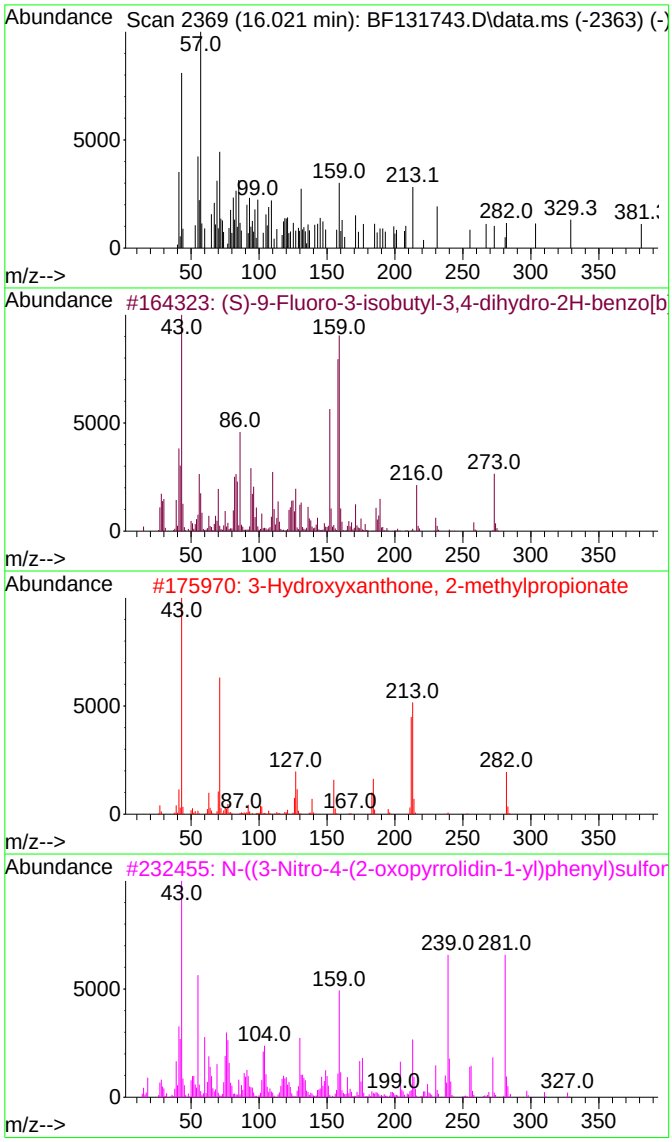
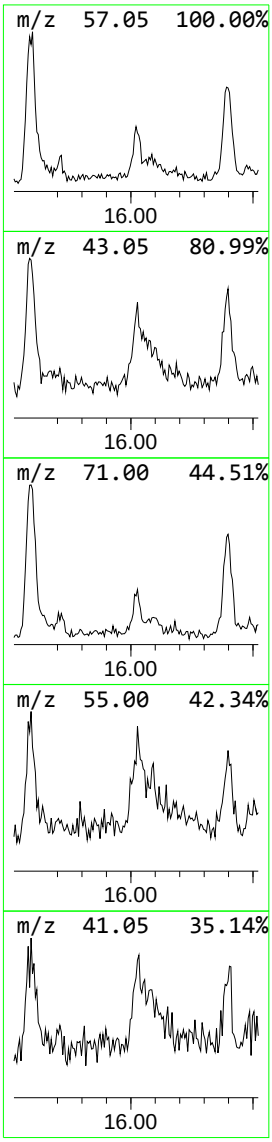
Peak Number 9 unknown16.021 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.021	6.03 ng	138510	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	(S)-9-Fluoro-3-isobutyl-3,4-dihy...	273	C12H16FNO3S	1257313-65-7	11
2	3-Hydroxyxanthone, 2-methylpropi...	282	C17H14O4	1000462-85-1	9
3	N-((3-Nitro-4-(2-oxopyrrolidin-1...	327	C12H13N3O6S	1000497-89-0	9
4	1,3,4-Thiadiazole, 2-acetylamino...	315	C14H13N5O2S	331246-48-1	9
5	4-Acetyl-1-(3-ethoxypropyl)-3-hy...	303	C17H21NO4	1000387-64-4	9





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Data File : BF131743.D
Acq On : 21 Dec 2022 13:26
Operator : CG\JU
Sample : N6100-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-303-20221215

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

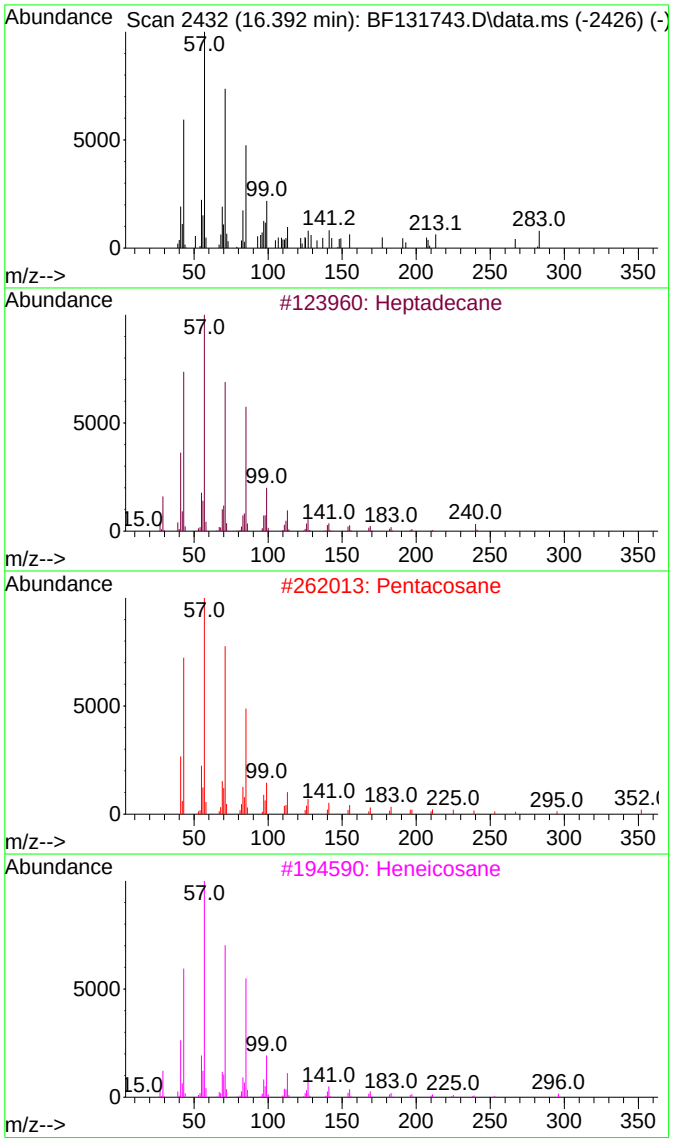
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

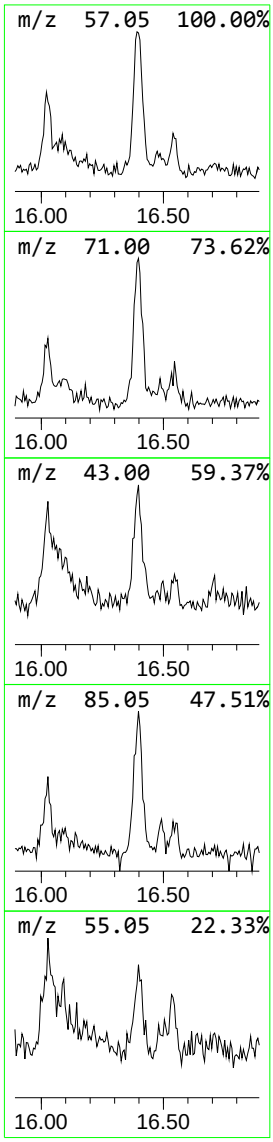
****

Peak Number 10 Heptadecane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.392	2.68 ng	61658	Perylene-d12	15.551

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	86
2	Pentacosane	352	C25H52	000629-99-2	83
3	Heneicosane	296	C21H44	000629-94-7	83
4	Hentriacontane	437	C31H64	000630-04-6	83
5	Eicosane	282	C20H42	000112-95-8	80





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF122122\
Data File : BF131743.D
Acq On : 21 Dec 2022 13:26
Operator : CG\JU
Sample : N6100-03
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SP-303-20221215

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122022.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
Butane, 2-metho...	2.116	66.9	ng	1690770	1	6.863	505146	20.0
2-Pentanone, 4-...	5.063	10.0	ng	253614	1	6.863	505146	20.0
Benzenamine, 2,...	11.475	2.5	ng	101838	4	11.410	819281	20.0
Octadecane, 1-c...	12.204	2.8	ng	112604	4	11.410	819281	20.0
Tetracosane	13.522	4.6	ng	121907	5	14.057	534241	20.0
Triphenylphosph...	14.151	8.4	ng	223842	5	14.057	534241	20.0
Heneicosane	14.286	5.4	ng	143459	5	14.057	534241	20.0
Eicosane	14.916	4.1	ng	93233	6	15.551	459728	20.0
unknown16.021	16.021	6.0	ng	138510	6	15.551	459728	20.0
Heptadecane	16.392	2.7	ng	61658	6	15.551	459728	20.0