LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137012.D
Acq On : 10 Jan 2024 10:55
Operator : CG\JU
Sample : PB158316BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158316BL

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-BF122023.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF137012.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.069	502	507	519	rBV	44224	75599	1.92%	0.363%
2	5.446	566	571	574	rBV	2553444	2586964	65.77%	12.412%
3	6.445	735	741	744	rBV	2258695	2609266	66.34%	12.519%
4	6.781	795	798	802	rBV	516177	464869	11.82%	2.230%
5	7.351	889	895	898	rBV	1509359	1753290	44.58%	8.412%
6	8.063	1011	1016	1019	rBV	643696	626958	15.94%	3.008%
7	9.145	1193	1200	1203	rBV	3315212	3324391	84.52%	15.950%
8	9.822	1309	1315	1318	rBV	770104	730920	18.58%	3.507%
9	10.622	1446	1451	1454	rBV	2035800	1974348	50.20%	9.473%
10	11.316	1565	1569	1572	rBV	1054345	841816	21.40%	4.039%
11	12.922	1836	1842	1845	rBV	3507510	3933147	100.00%	18.871%
12	13.974	2017	2021	2029	rVB	798258	722202	18.36%	3.465%
13	14.745	2147	2152	2158	rBV	66793	75789	1.93%	0.364%
14	15.092	2207	2211	2217	rVB	82417	94711	2.41%	0.454%
15	15.468	2269	2275	2283	rVB	424133	654469	16.64%	3.140%
16	15.927	2348	2353	2360	rVB2	74982	126880	3.23%	0.609%
17	16.451	2436	2442	2450	rBV2	59858	114231	2.90%	0.548%
18	17.068	2541	2547	2553	rVB3	34159	70509	1.79%	0.338%
19	17.792	2666	2670	2681	rVB4	24694	62106	1.58%	0.298%

Sum of corrected areas: 20842465

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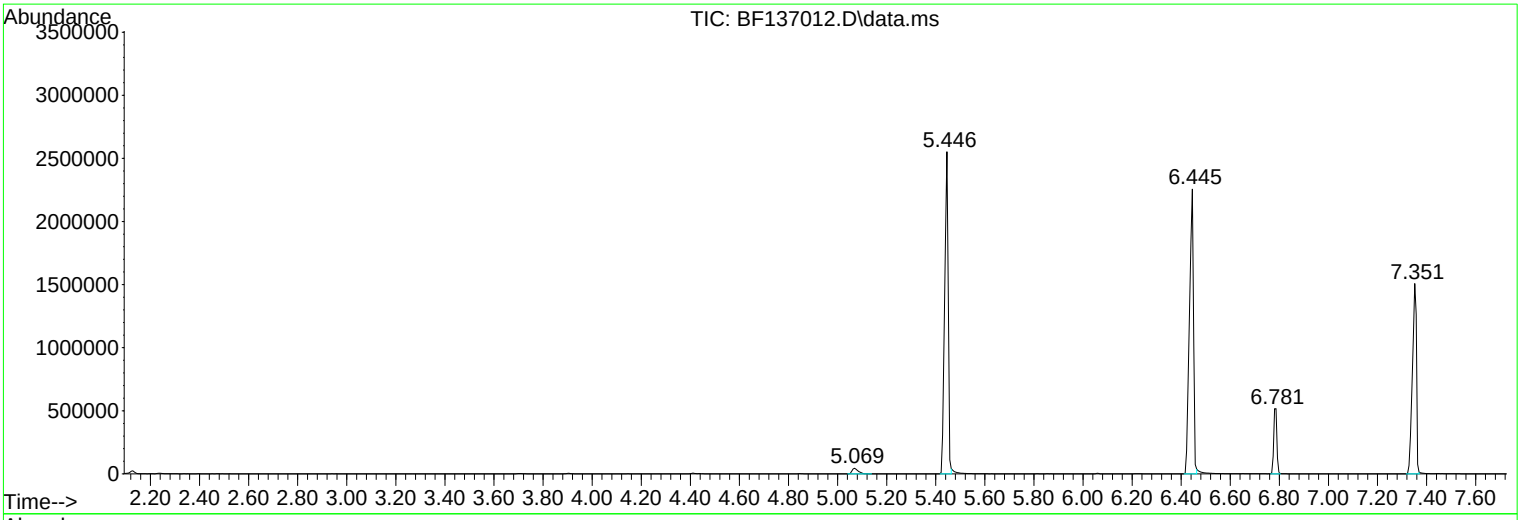
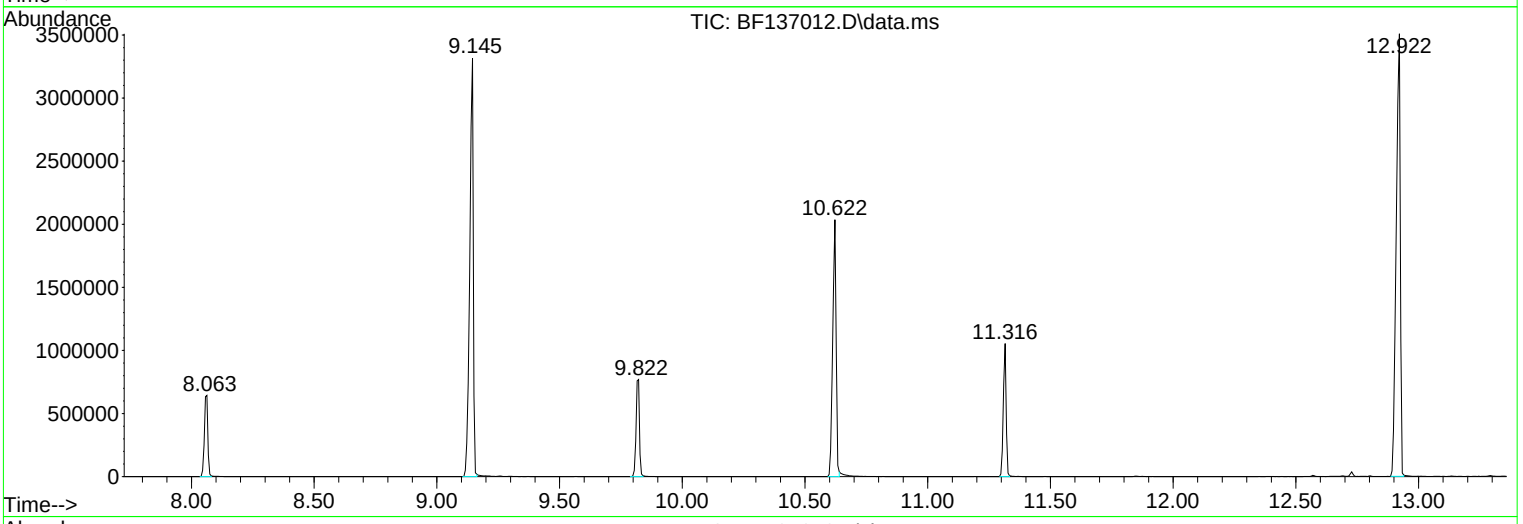
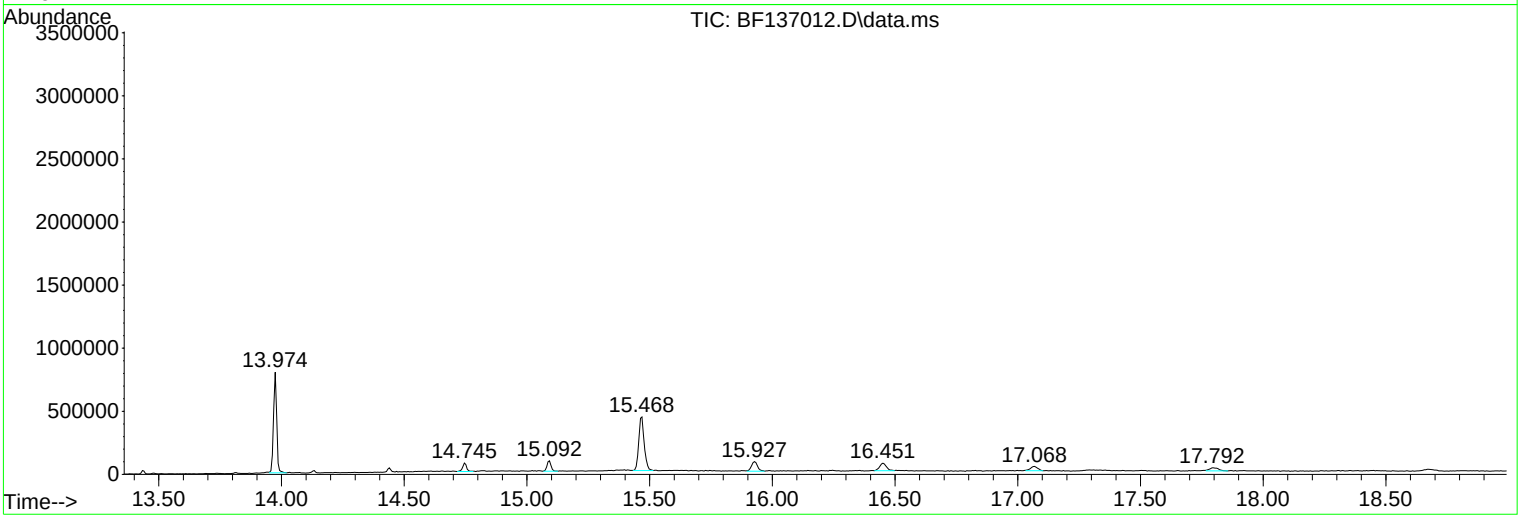
Instrument :
BNA_F
ClientSampleId :
PB158316BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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







Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137012.D
Acq On : 10 Jan 2024 10:55
Operator : CG\JU
Sample : PB158316BL
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Instrument :
BNA_F
ClientSampleId :
PB158316BL

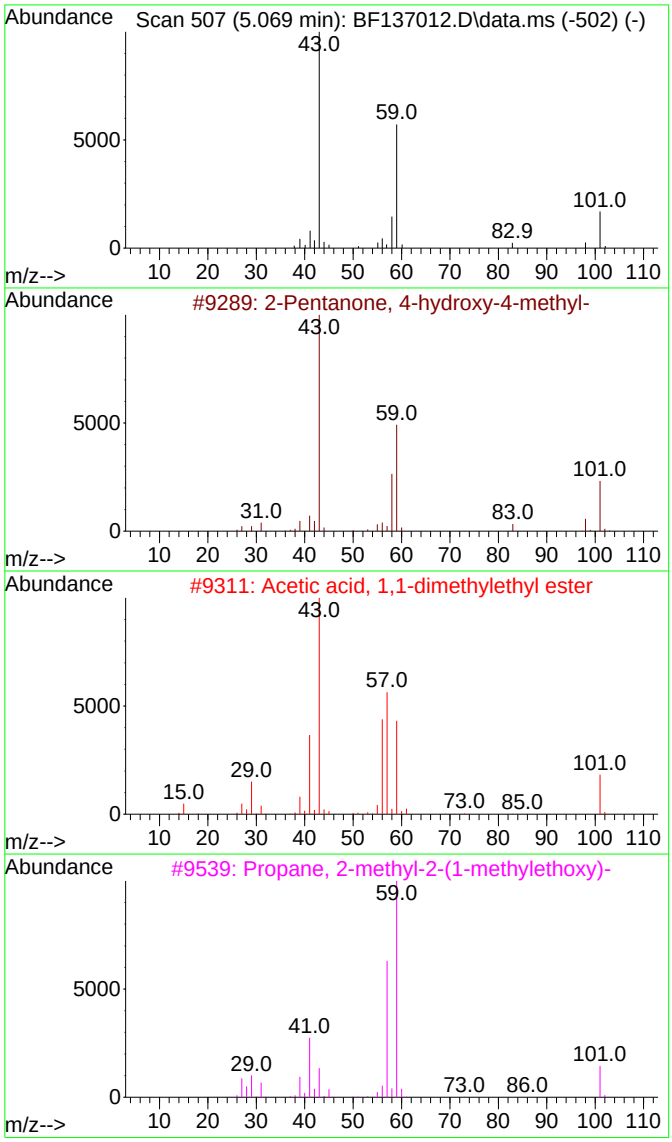
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

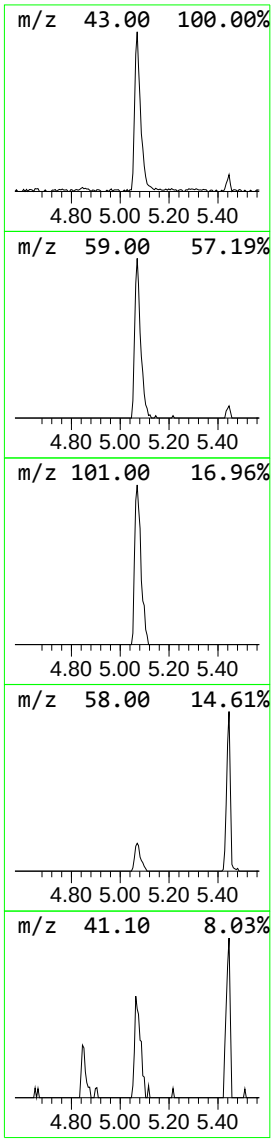
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	3.25 ng	75599	1,4-Dichlorobenzene-d4	6.787

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
4	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
5	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12





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Sample : PB158316BL
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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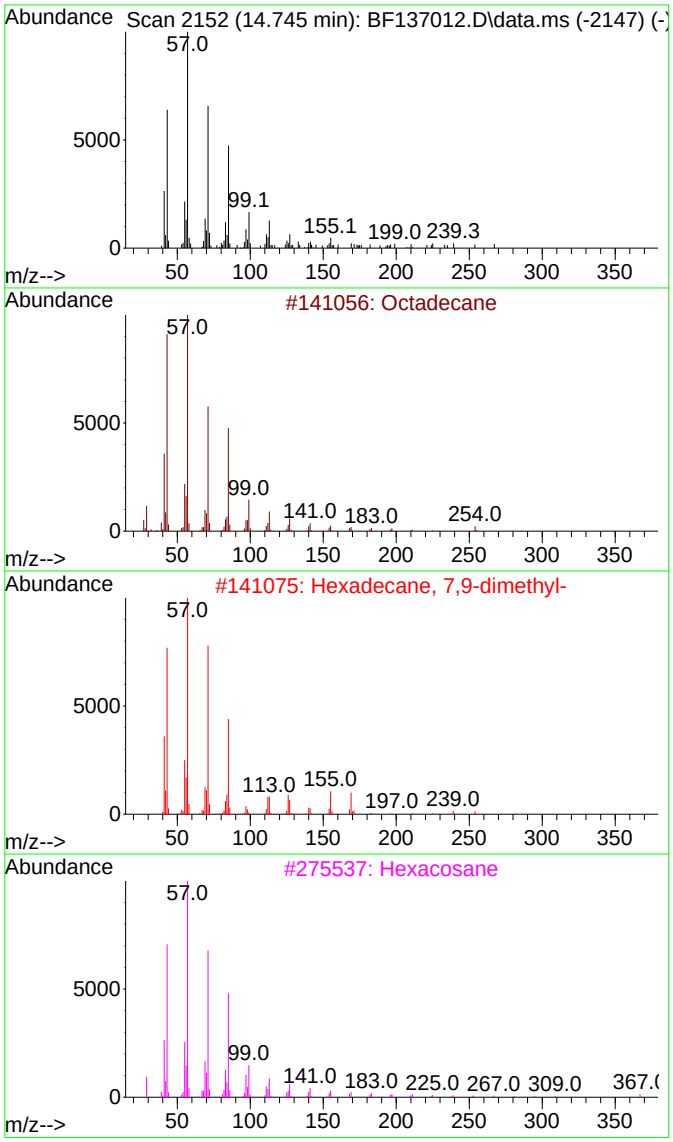
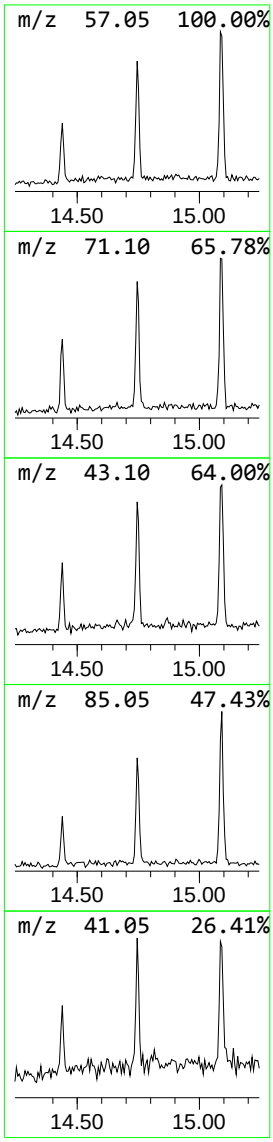
Peak Number 2 Octadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.745	2.32 ng	75789	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecane	254	C18H38	000593-45-3	94
2	Hexadecane, 7,9-dimethyl-	254	C18H38	021164-95-4	91
3	Hexacosane	366	C26H54	000630-01-3	87
4	Pentacosane	352	C25H52	000629-99-2	87
5	Hentriacontane	437	C31H64	000630-04-6	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
Data File : BF137012.D
Acq On : 10 Jan 2024 10:55
Operator : CG\JU
Sample : PB158316BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158316BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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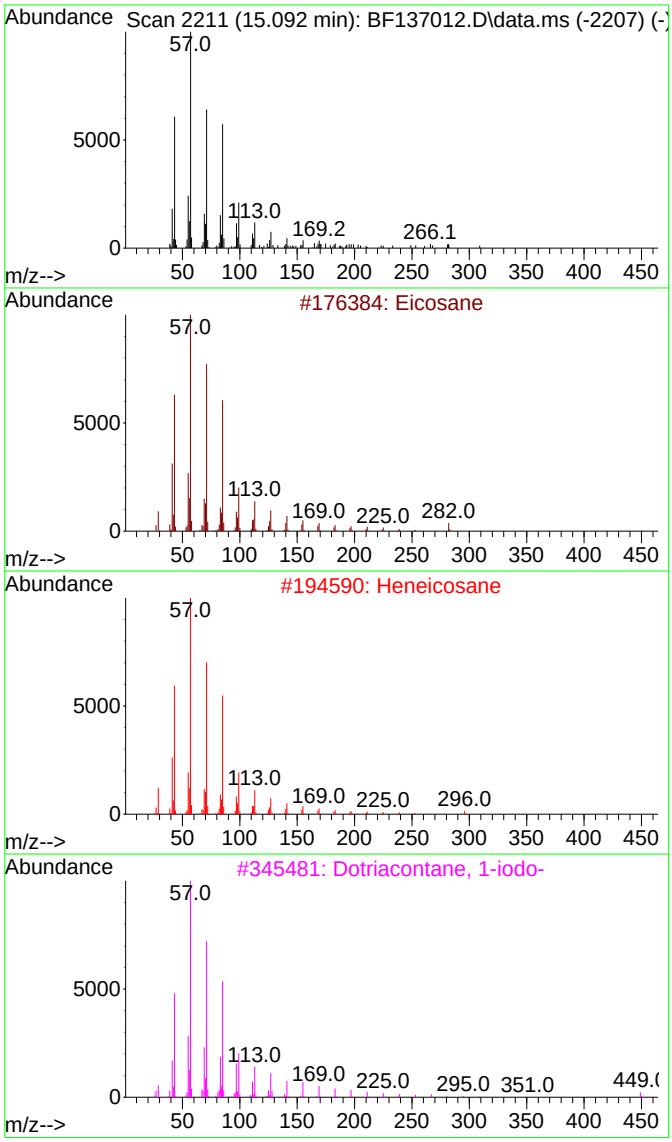
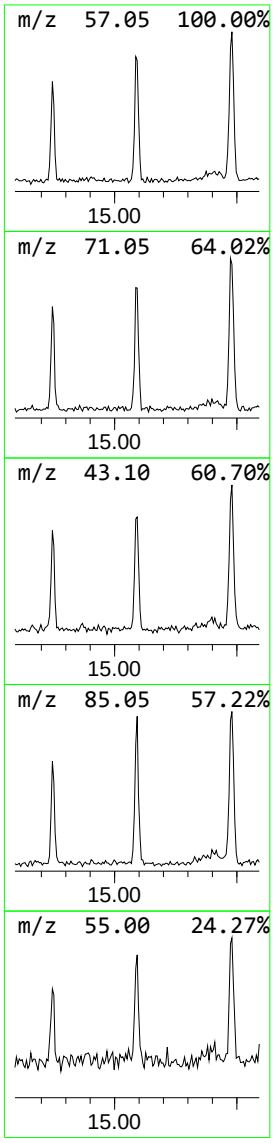
Peak Number 3 Eicosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.092	2.89 ng	94711	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	95
2	Heneicosane	296	C21H44	000629-94-7	90
3	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87
4	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
5	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87





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Data File : BF137012.D
Acq On : 10 Jan 2024 10:55
Operator : CG\JU
Sample : PB158316BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158316BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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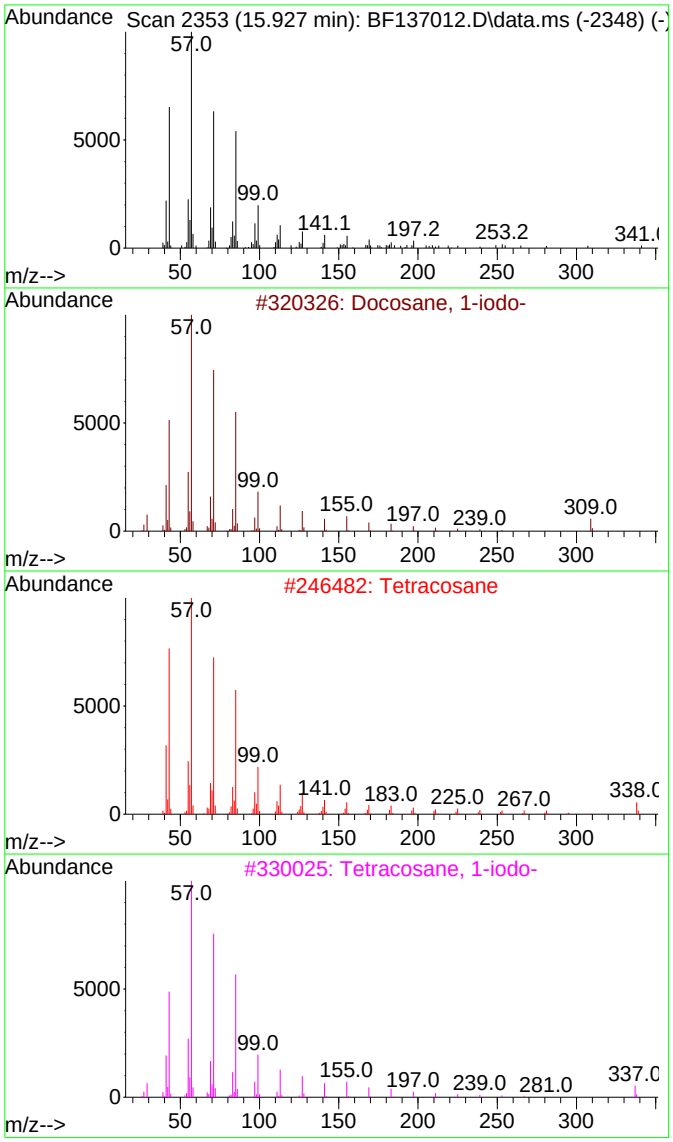
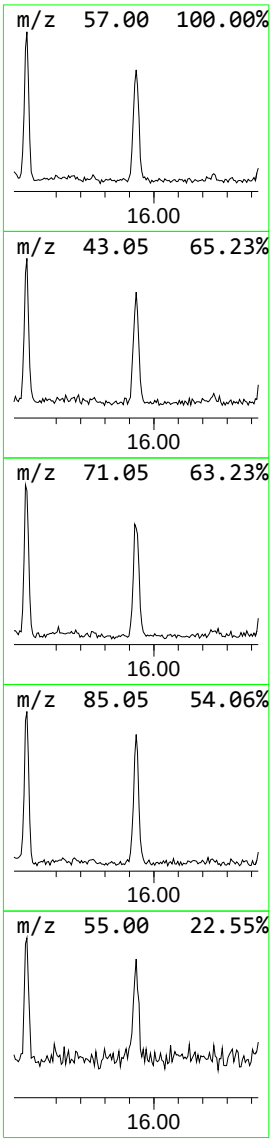
Peak Number 4 Docosane, 1-iodo- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.927	3.88 ng	126880	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	90
2	Tetracosane	338	C24H50	000646-31-1	87
3	Tetracosane, 1-iodo-	464	C24H49I	1000406-32-0	87
4	Triacontane	422	C30H62	000638-68-6	87
5	Eicosane, 2-methyl-	296	C21H44	001560-84-5	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF011024\
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Acq On : 10 Jan 2024 10:55
Operator : CG\JU
Sample : PB158316BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158316BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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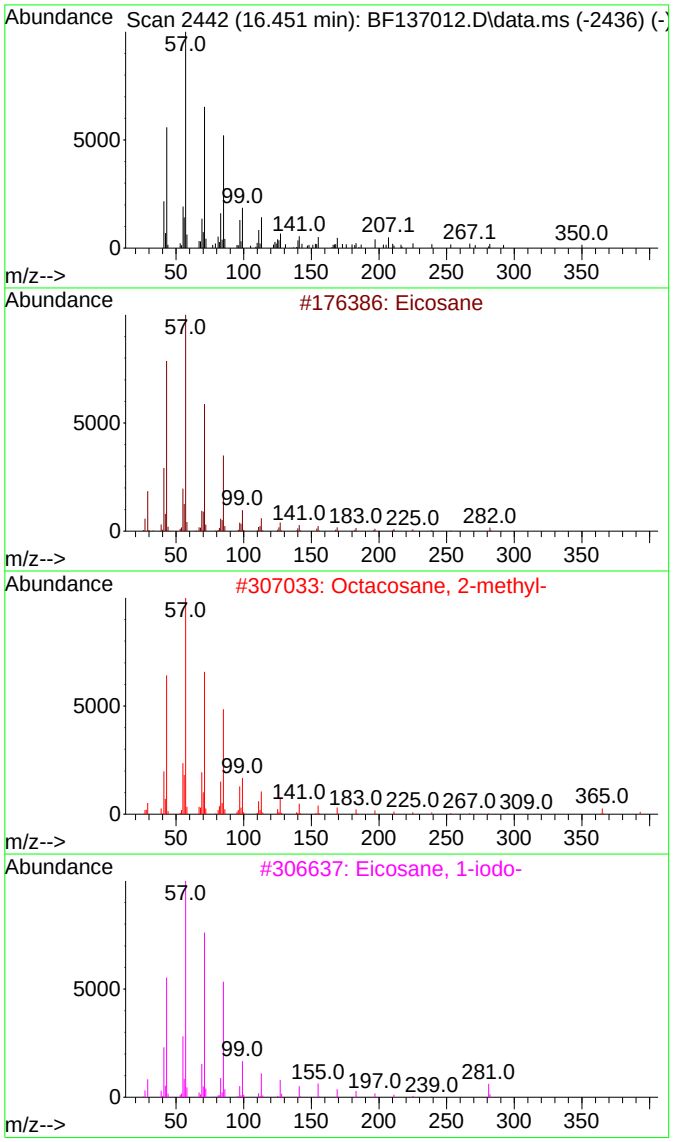
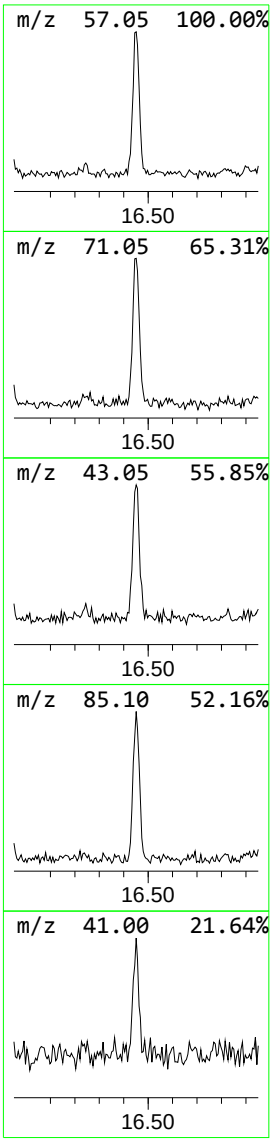
Peak Number 5 Octacosane, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.451	3.49 ng	114231	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
3	Eicosane, 1-iodo-	408	C20H41I	1000406-31-8	87
4	Nonadecane, 2,3-dimethyl-	296	C21H44	075163-99-4	87
5	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87





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Sample : PB158316BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PB158316BL

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF122023.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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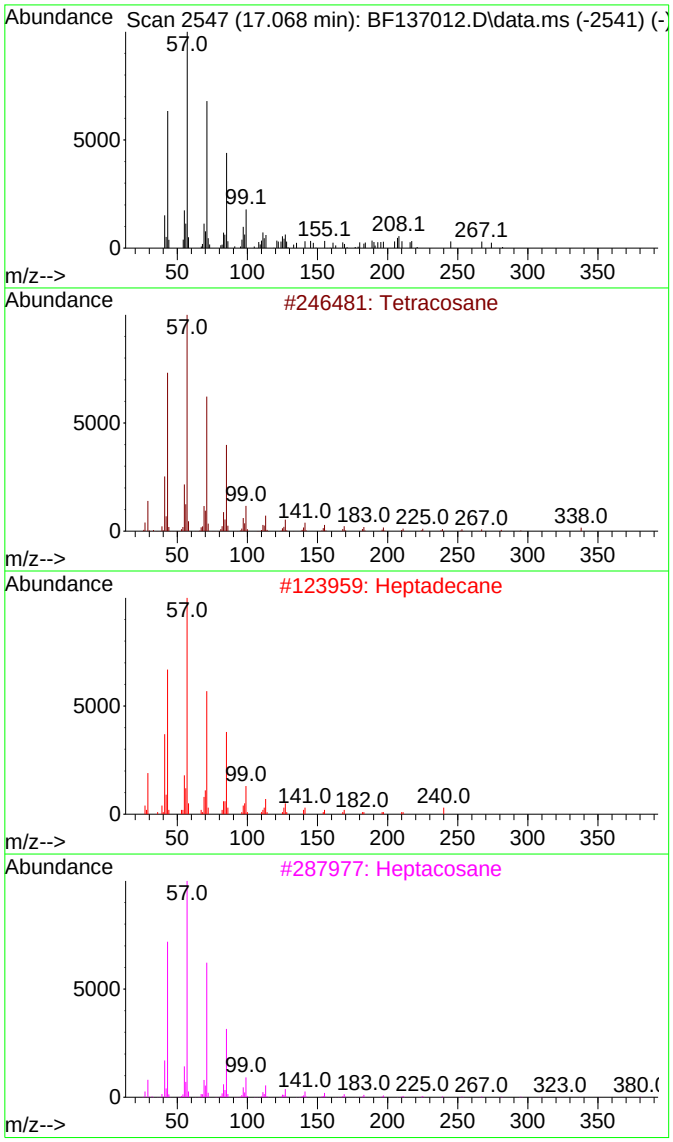
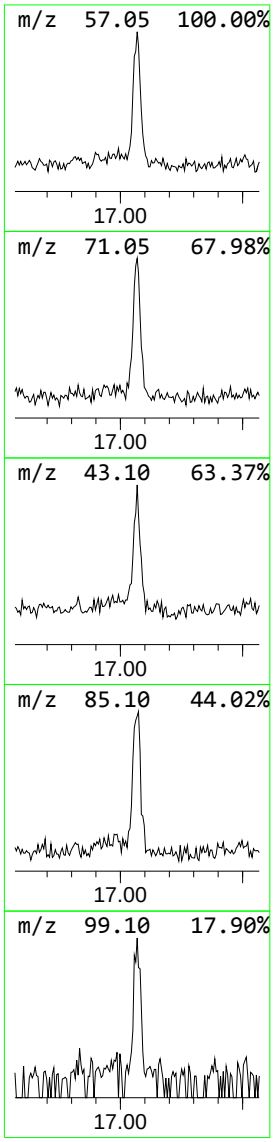
Peak Number 6 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.068	2.15 ng	70509	Perylene-d12	15.463

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	83
2	Heptadecane	240	C17H36	000629-78-7	80
3	Heptacosane	380	C27H56	000593-49-7	80
4	Nonadecane	268	C19H40	000629-92-5	74
5	Eicosane	282	C20H42	000112-95-8	74





Tentatively Identified Compound (LSC) summary

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ClientSampleId :
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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
2-Pentanone, 4-...	5.069	3.3	ng	75599	1	6.787	464869	20.0
Octadecane	14.745	2.3	ng	75789	6	15.463	654469	20.0
Eicosane	15.092	2.9	ng	94711	6	15.463	654469	20.0
Docosane, 1-iodo-	15.927	3.9	ng	126880	6	15.463	654469	20.0
Octacosane, 2-m...	16.451	3.5	ng	114231	6	15.463	654469	20.0
Tetracosane	17.068	2.1	ng	70509	6	15.463	654469	20.0