LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129244.D
Acq On : 15 Jul 2022 18:16
Operator : CG\JU
Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

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-BF071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF129244.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.145	483	486	496	rVB	107964	133609	1.61%	0.216%
2	5.522	544	550	553	rBV	6913743	7023189	84.59%	11.335%
3	6.522	714	720	723	rBV	6169153	7236047	87.16%	11.679%
4	6.892	780	783	787	rVB	1764526	1575031	18.97%	2.542%
5	7.457	874	879	882	rBV	4435820	4767075	57.42%	7.694%
6	8.175	997	1001	1005	rBV	2207395	2145337	25.84%	3.462%
7	9.257	1179	1185	1188	rBV	8231381	8302317	100.00%	13.400%
8	9.586	1236	1241	1247	rBV2	70715	99555	1.20%	0.161%
9	9.904	1290	1295	1297	rBV2	77793	91270	1.10%	0.147%
10	9.933	1297	1300	1304	rVB	2689006	2367728	28.52%	3.821%
11	10.245	1348	1353	1356	rBV2	73187	147110	1.77%	0.237%
12	10.727	1430	1435	1438	rBV	5656562	5241212	63.13%	8.459%
13	10.833	1450	1453	1461	rVB4	71548	123669	1.49%	0.200%
14	11.427	1550	1554	1556	rBV	2568169	2364142	28.48%	3.816%
15	11.445	1556	1557	1560	rVV	580124	463961	5.59%	0.749%
16	11.498	1564	1566	1568	rVB	145293	119934	1.44%	0.194%
17	11.810	1616	1619	1621	rBV	346548	325343	3.92%	0.525%
18	11.945	1640	1642	1645	rBV2	300176	316492	3.81%	0.511%
19	12.651	1759	1762	1771	rVB	1290607	1567613	18.88%	2.530%
20	12.874	1797	1800	1803	rVB	1086834	869210	10.47%	1.403%
21	13.016	1819	1824	1827	rVB	7733112	7717118	92.95%	12.455%
22	13.086	1832	1836	1840	rVB2	64335	106211	1.28%	0.171%
23	13.198	1853	1855	1857	rVB	106943	86295	1.04%	0.139%
24	13.227	1857	1860	1863	rBV	113932	90444	1.09%	0.146%
25	13.574	1915	1919	1925	rBV	177471	206747	2.49%	0.334%
26	13.704	1937	1941	1947	rVB	80825	96317	1.16%	0.155%
27	13.898	1972	1974	1979	rVB2	307482	296517	3.57%	0.479%
28	14.068	1998	2003	2005	rBV2	1810304	1837759	22.14%	2.966%
29	14.092	2005	2007	2013	rVB	393757	354808	4.27%	0.573%
30	14.157	2015	2018	2025	rVB2	188788	250560	3.02%	0.404%
31	14.215	2025	2028	2032	rBV	391005	329734	3.97%	0.532%
32	14.521	2077	2080	2084	rBV	409034	353344	4.26%	0.570%
33	14.833	2129	2133	2138	rVB	264960	288265	3.47%	0.465%
34	14.986	2155	2159	2163	rVB	151712	161476	1.94%	0.261%
35	15.115	2177	2181	2185	rBV	271601	436674	5.26%	0.705%
36	15.174	2188	2191	2197	rVB	311230	377224	4.54%	0.609%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129244.D
Acq On : 15 Jul 2022 18:16
Operator : CG\JU
Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

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-BF071522.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

37	15.427	2230	2234	2240	rVB	174601	232604	2.80%	0.375%
38	15.492	2241	2245	2251	rVB	239324	302684	3.65%	0.489%
39	15.557	2251	2256	2268	rVB	1150417	1608848	19.38%	2.597%
40	15.774	2290	2293	2298	rVB4	61260	83835	1.01%	0.135%
41	16.009	2328	2333	2343	rBV	336819	535713	6.45%	0.865%
42	16.533	2417	2422	2428	rVB	74551	126229	1.52%	0.204%
43	17.051	2505	2510	2520	rVV2	116032	235444	2.84%	0.380%
44	17.139	2520	2525	2533	rVB	94938	196569	2.37%	0.317%
45	17.509	2583	2588	2597	rVB	104862	216197	2.60%	0.349%
46	18.709	2790	2792	2804	rVB7	59170	152436	1.84%	0.246%

Sum of corrected areas: 61959896

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129244.D
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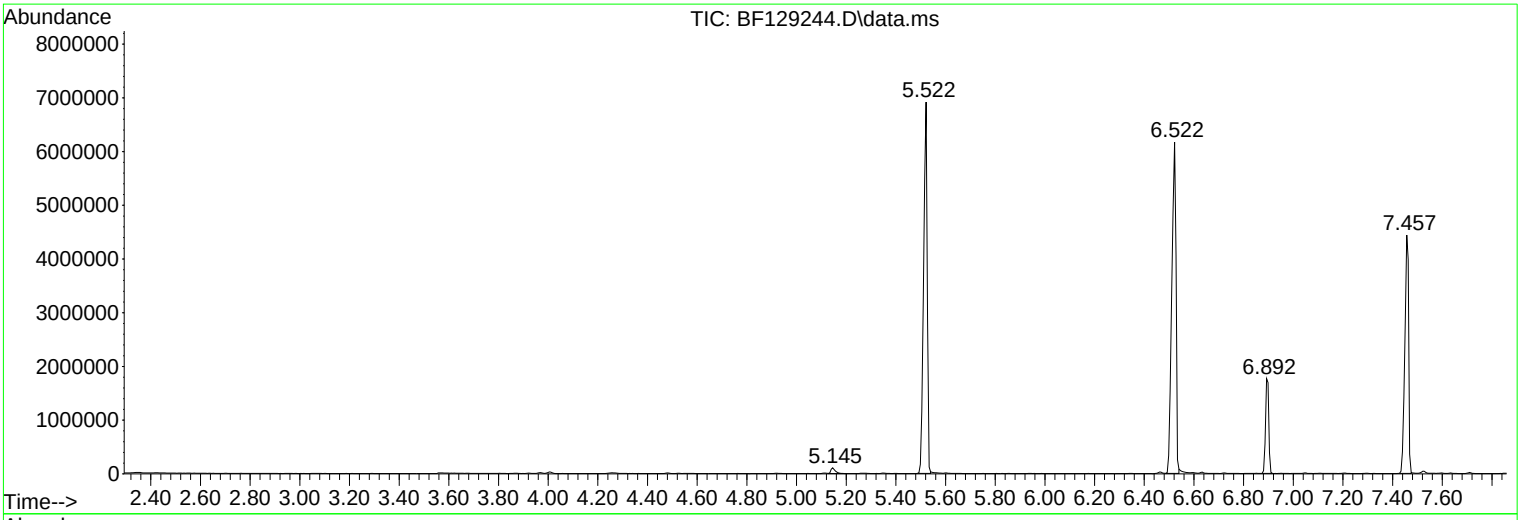
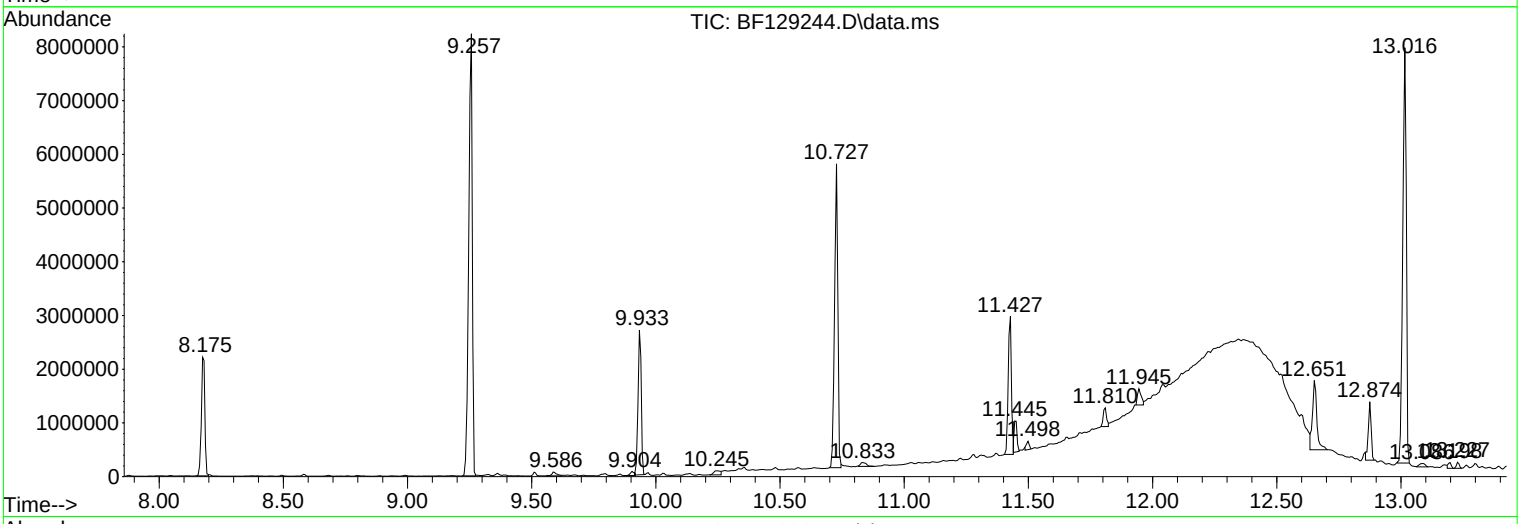
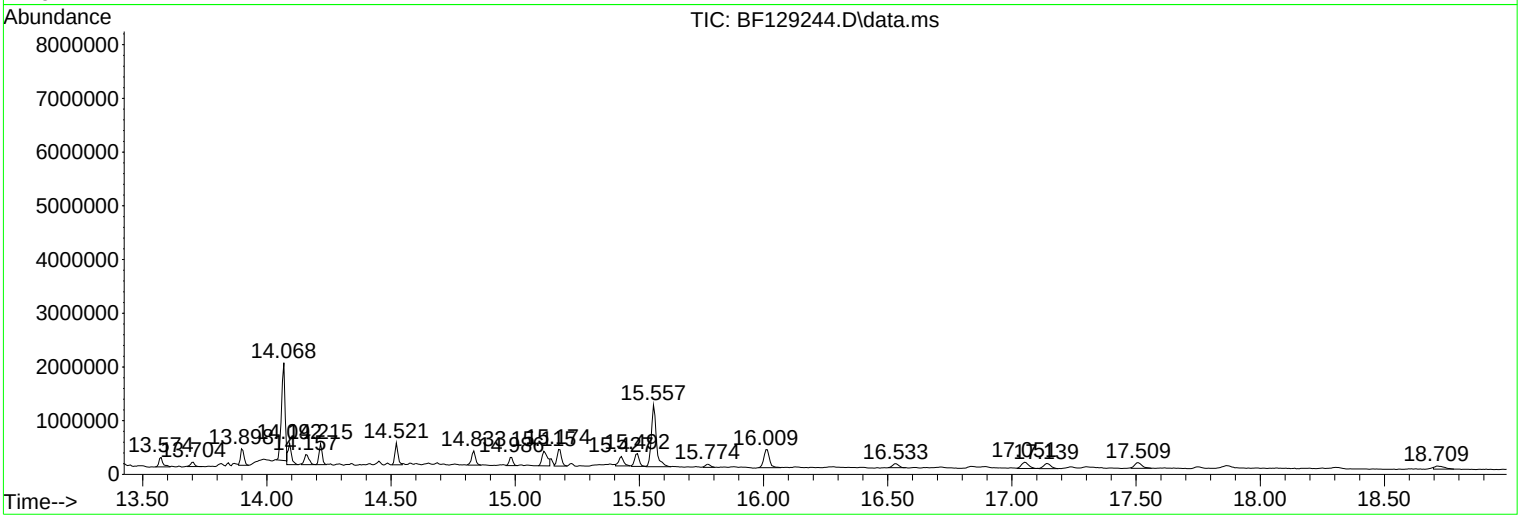
Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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\BF071522\
Data File : BF129244.D
Acq On : 15 Jul 2022 18:16
Operator : CG\JU
Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

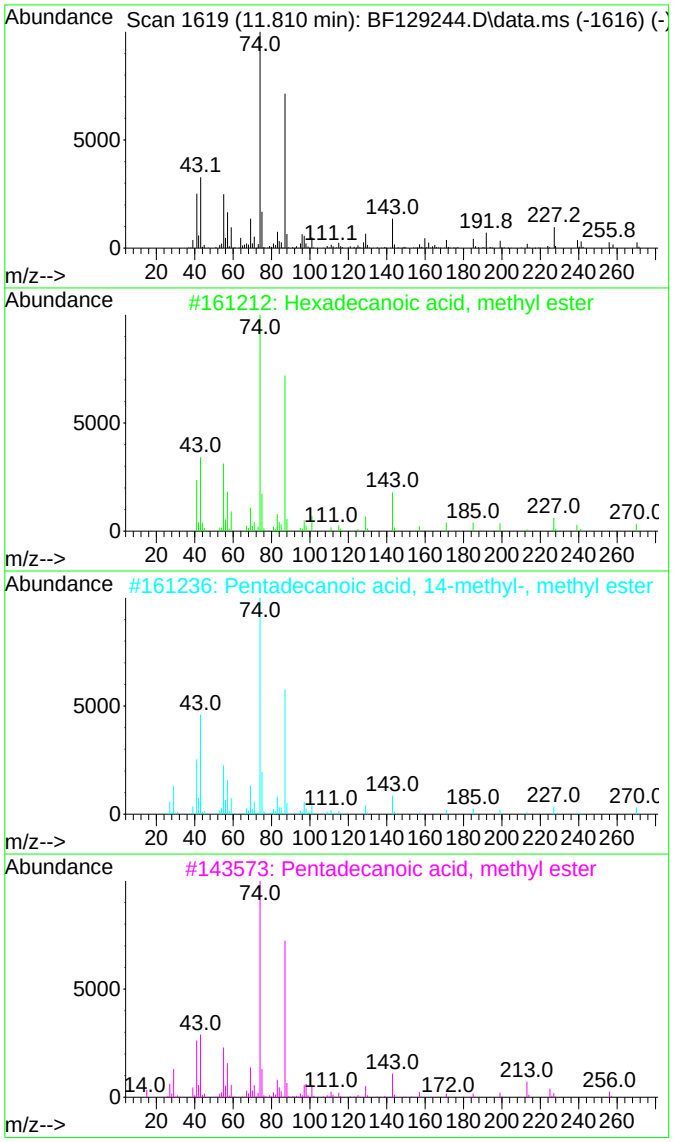
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

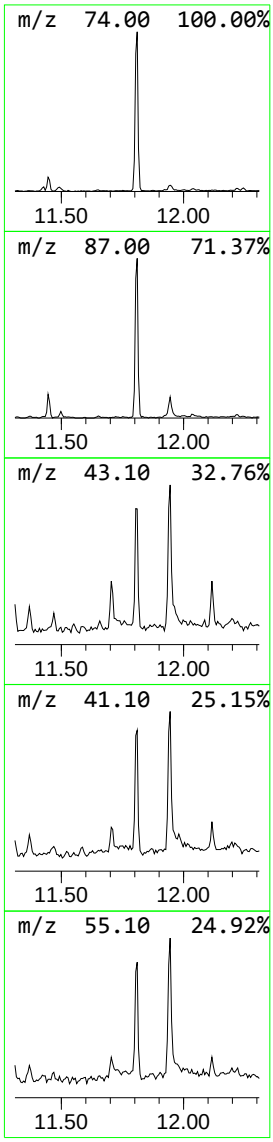
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.810	2.75 ng	325343	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester	270	C17H34O2	000112-39-0	98
2	Pentadecanoic acid, 14-methyl-, ...	270	C17H34O2	005129-60-2	96
3	Pentadecanoic acid, methyl ester	256	C16H32O2	007132-64-1	91
4	Methyl 11-methyl-dodecanoate	228	C14H28O2	1000336-45-1	72
5	Methyl tetradecanoate	242	C15H30O2	000124-10-7	72





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129244.D
Acq On : 15 Jul 2022 18:16
Operator : CG\JU
Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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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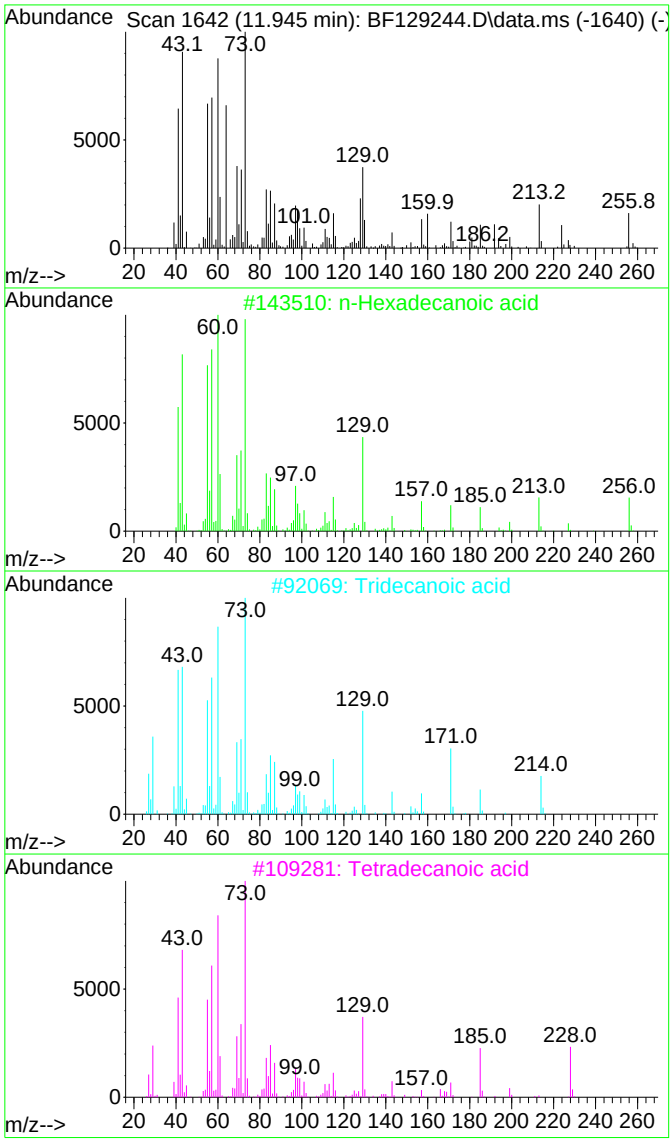
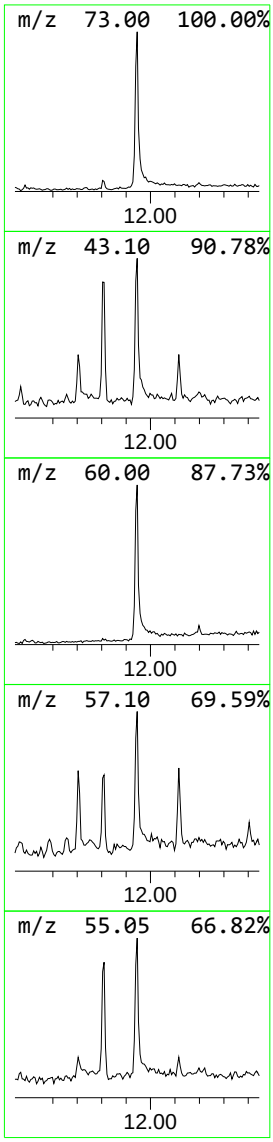
Peak Number 2 n-Hexadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.945	2.68 ng	316492	Phenanthrene-d10	11.427

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2	Tridecanoic acid	214	C13H26O2	000638-53-9	84
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	49
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	42
5	n-Decanoic acid	172	C10H20O2	000334-48-5	35





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129244.D
Acq On : 15 Jul 2022 18:16
Operator : CG\JU
Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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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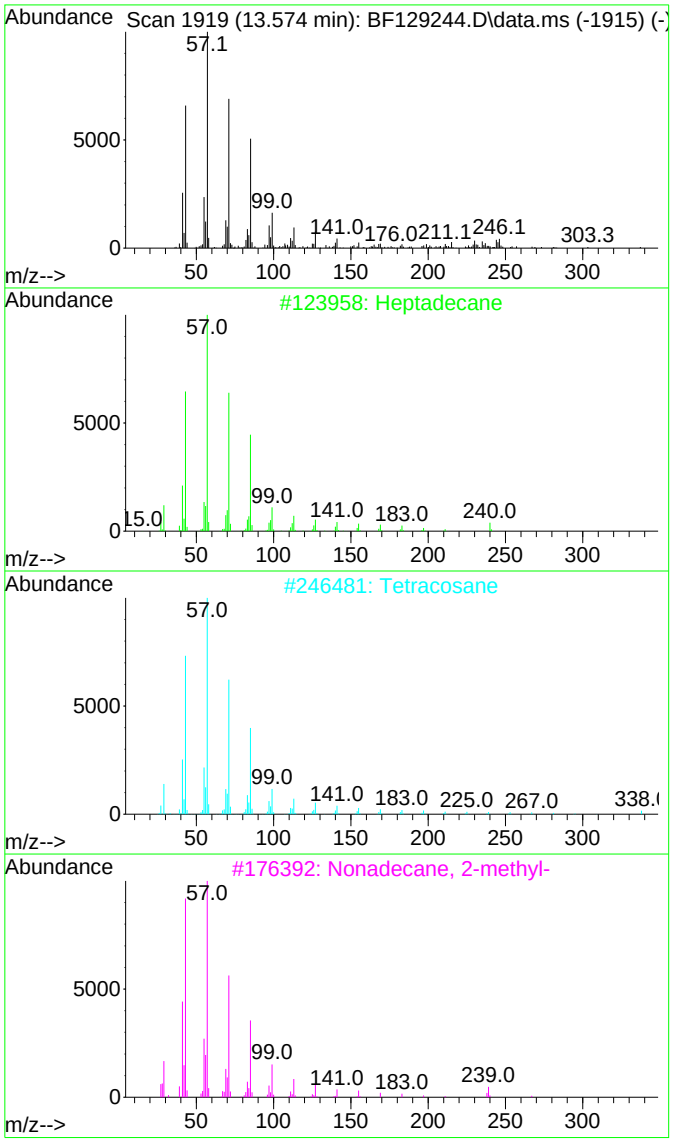
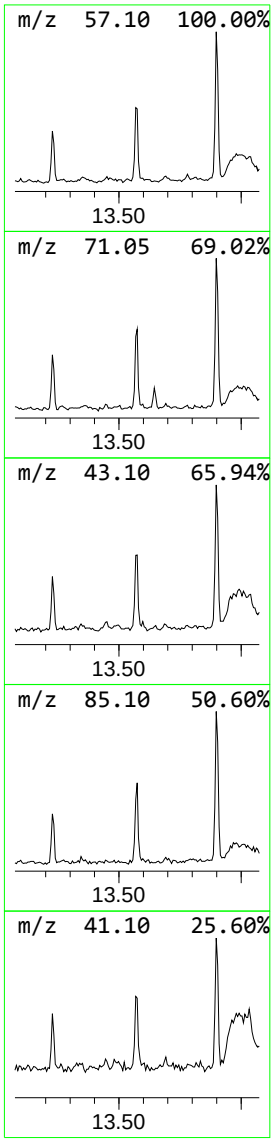
Peak Number 3 Heptadecane Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.574	2.25 ng	206747	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecane	240	C17H36	000629-78-7	94
2	Tetracosane	338	C24H50	000646-31-1	83
3	Nonadecane, 2-methyl-	282	C20H42	001560-86-7	83
4	Tetradecane, 2,6,10-trimethyl-	240	C17H36	014905-56-7	83
5	4-Methylheneicosane	310	C22H46	025117-29-7	80





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129244.D
Acq On : 15 Jul 2022 18:16
Operator : CG\JU
Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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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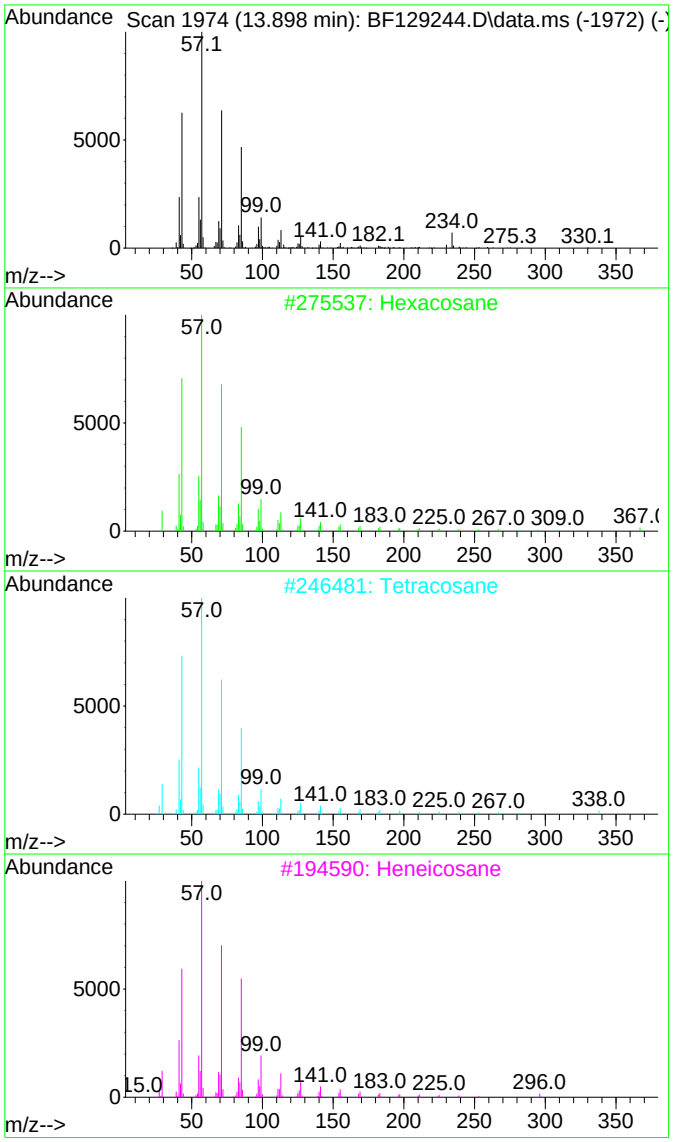
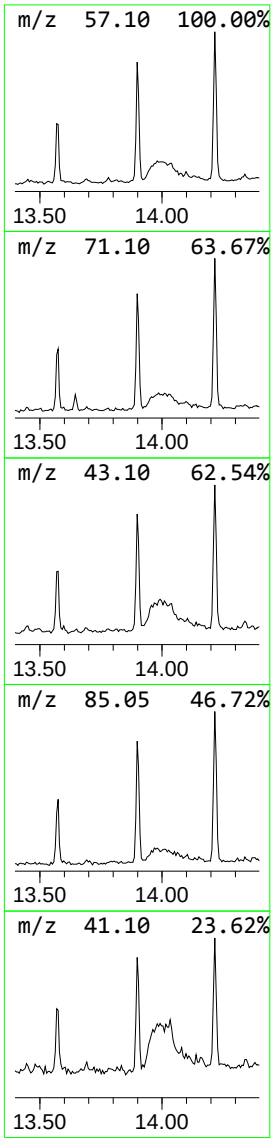
Peak Number 4 Hexacosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.898	3.23 ng	296517	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	90
2	Tetracosane	338	C24H50	000646-31-1	87
3	Heneicosane	296	C21H44	000629-94-7	87
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	87
5	Nonadecane	268	C19H40	000629-92-5	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129244.D
Acq On : 15 Jul 2022 18:16
Operator : CG\JU
Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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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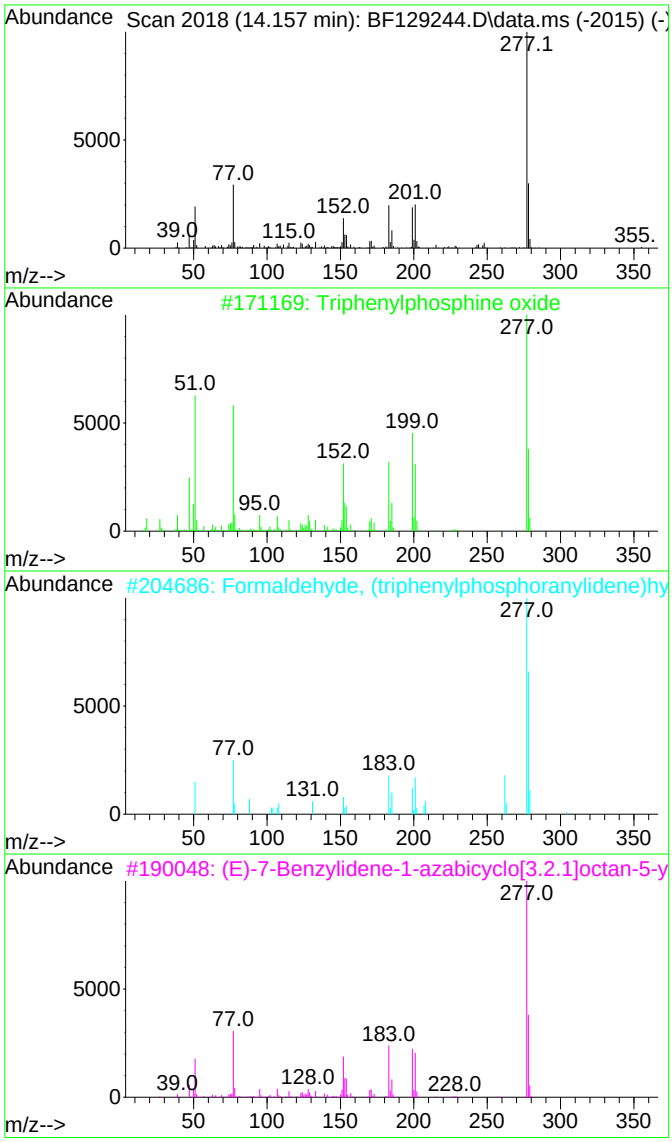
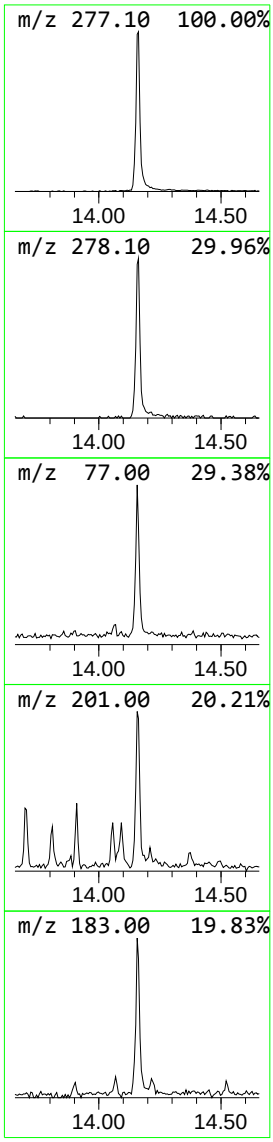
Peak Number 5 Triphenylphosphine oxide Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.157	2.73 ng	250560	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	91
2	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	56
3	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	49
4	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	43
5	Carbazol-1-one, 1,2,3,4-tetrahyd...	277	C18H15NO2	299962-12-2	38





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129244.D
Acq On : 15 Jul 2022 18:16
Operator : CG\JU
Sample : N3731-01
Misc :
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Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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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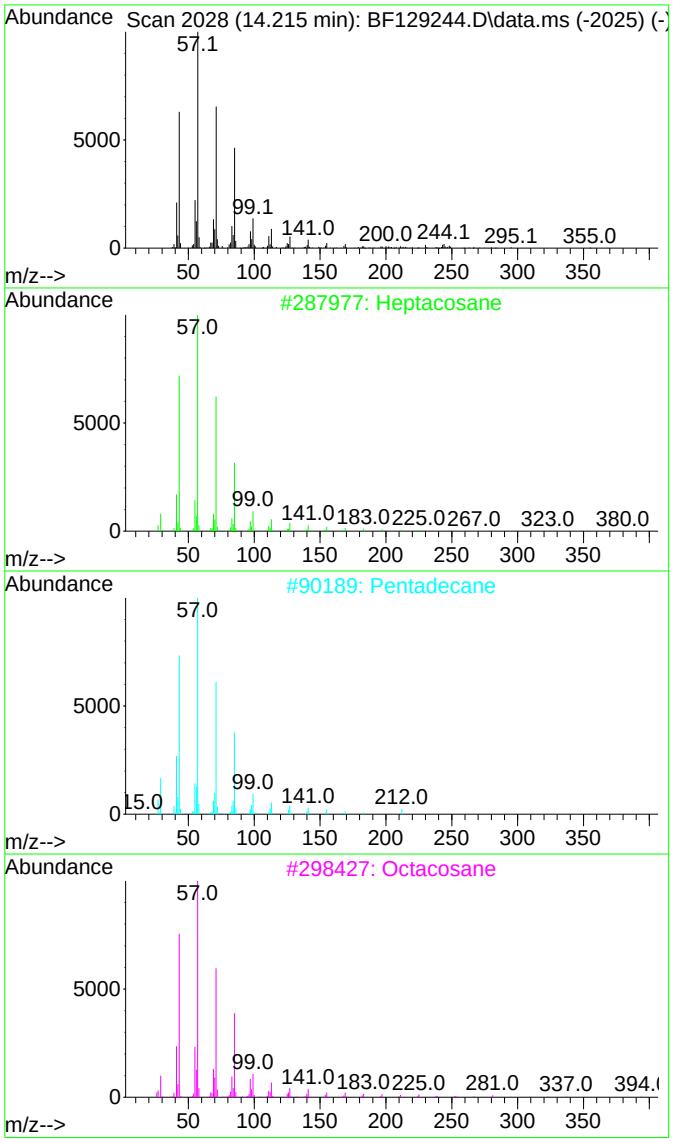
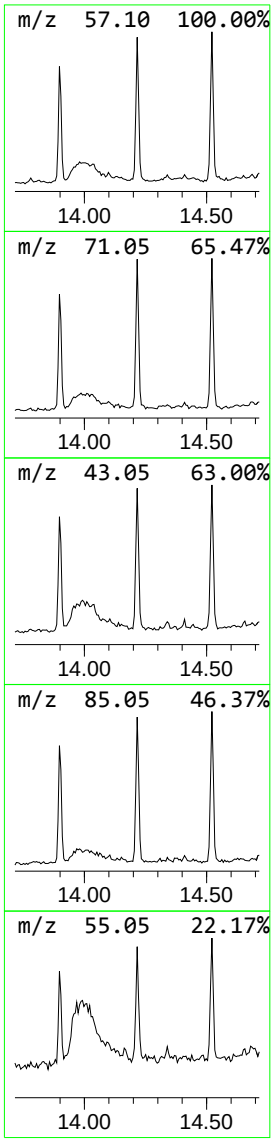
Peak Number 6 Heptacosane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.216	3.59 ng	329734	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Pentadecane	212	C15H32	000629-62-9	91
3	Octacosane	394	C28H58	000630-02-4	91
4	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	91
5	Hexacosane	366	C26H54	000630-01-3	91





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129244.D
Acq On : 15 Jul 2022 18:16
Operator : CG\JU
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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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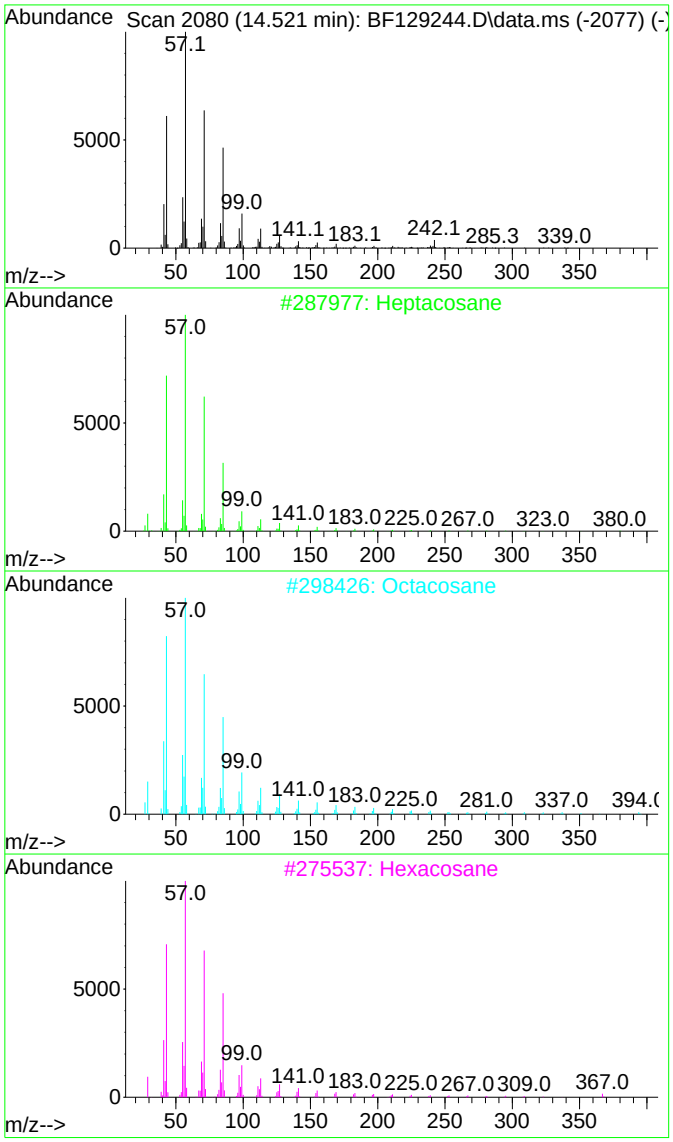
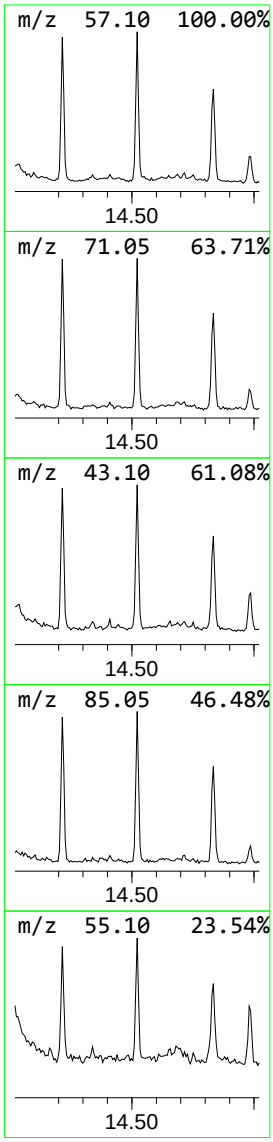
Peak Number 7 Octacosane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.521	3.85 ng	353344	Chrysene-d12	14.068

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	91
2	Octacosane	394	C28H58	000630-02-4	91
3	Hexacosane	366	C26H54	000630-01-3	91
4	Heneicosane	296	C21H44	000629-94-7	90
5	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	87





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129244.D
Acq On : 15 Jul 2022 18:16
Operator : CG\JU
Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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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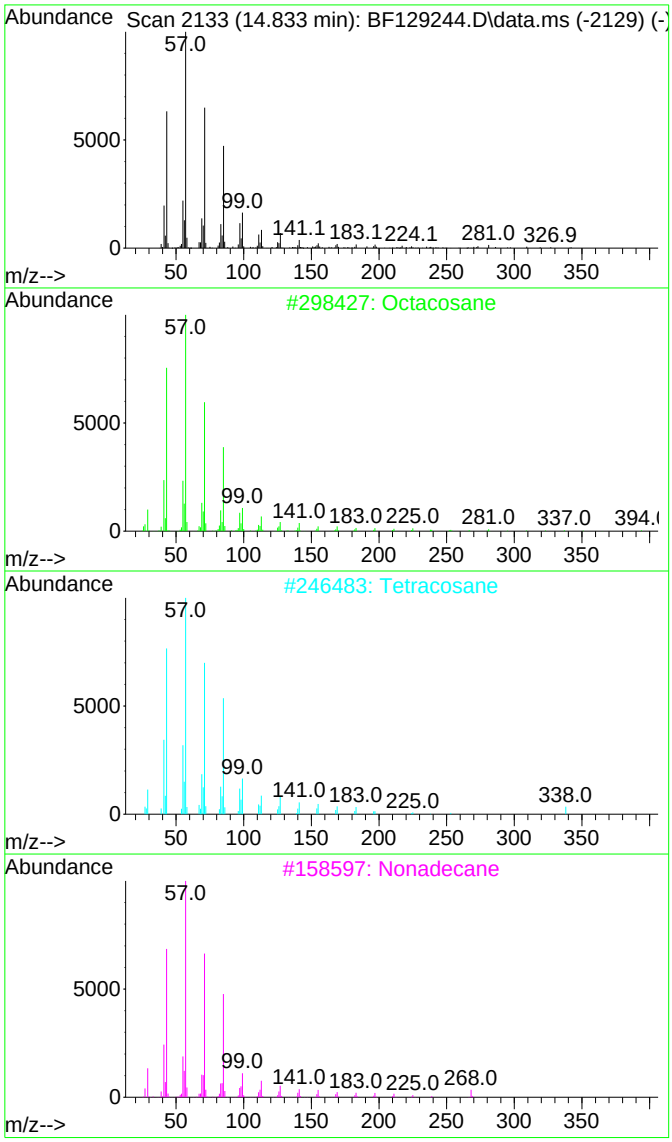
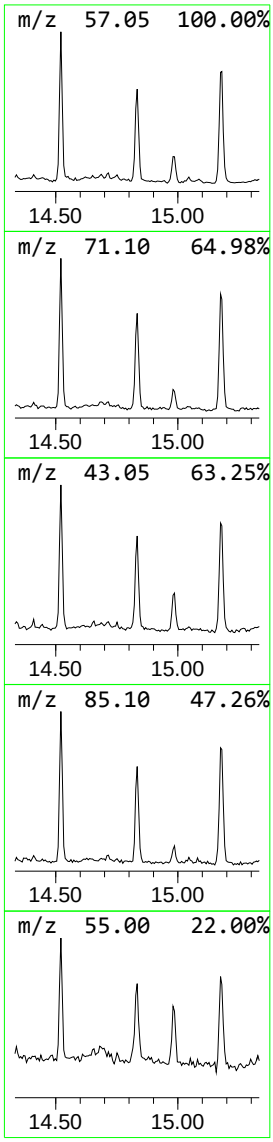
Peak Number 8 Tetracosane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.833	3.58 ng	288265	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane	394	C28H58	000630-02-4	91
2	Tetracosane	338	C24H50	000646-31-1	91
3	Nonadecane	268	C19H40	000629-92-5	87
4	Heptacosane	380	C27H56	000593-49-7	87
5	Heptadecane	240	C17H36	000629-78-7	86





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Data File : BF129244.D
Acq On : 15 Jul 2022 18:16
Operator : CG\JU
Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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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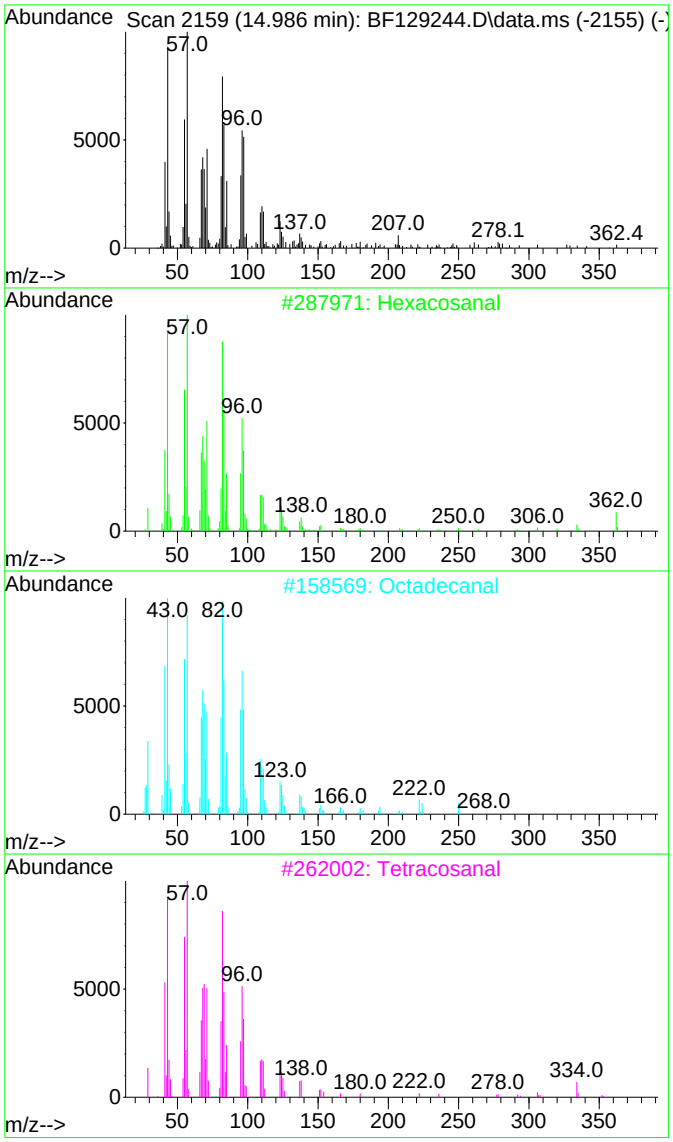
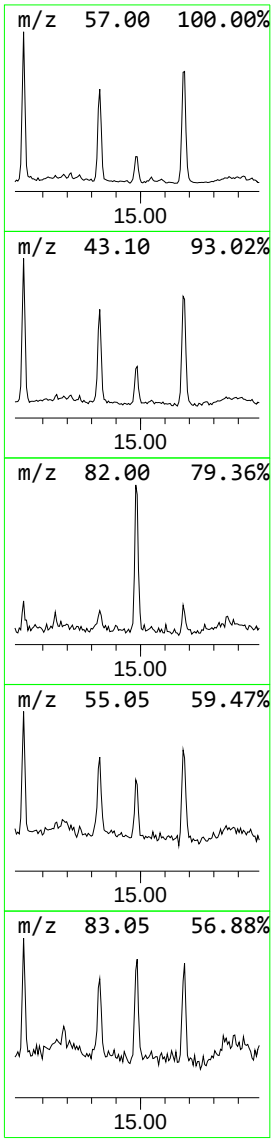
Peak Number 9 Hexacosanal Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.986	2.01 ng	161476	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosanal	380	C26H52O	026627-85-0	90
2	Octadecanal	268	C18H36O	000638-66-4	87
3	Tetracosanal	352	C24H48O	057866-08-7	87
4	Eicosanal-	296	C20H40O	002400-66-0	87
5	Heptadecanal	254	C17H34O	1000376-70-0	83





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Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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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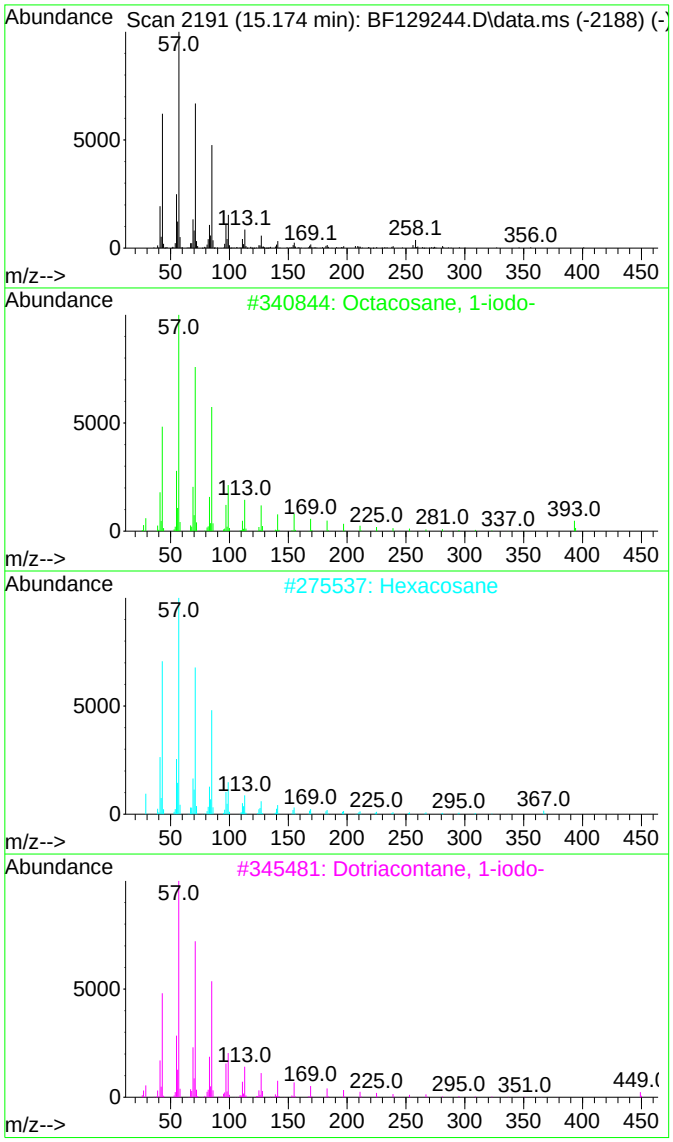
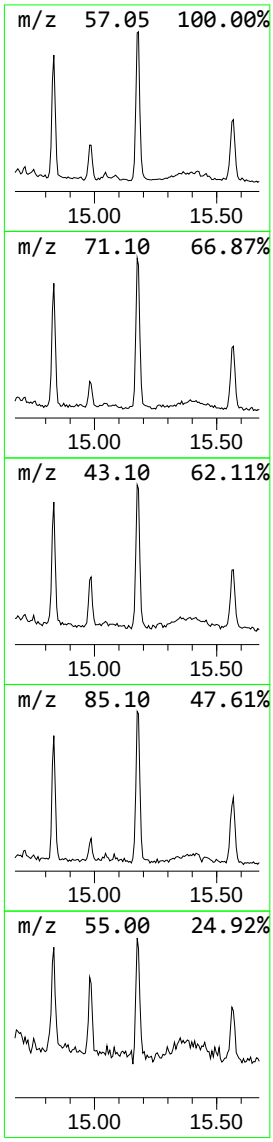
Peak Number 10 Octacosane, 1-iodo- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.174	4.69 ng	377224	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 1-iodo-	520	C28H57I	1000406-32-2	91
2	Hexacosane	366	C26H54	000630-01-3	90
3	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	90
4	Hexacosane, 1-iodo-	492	C26H53I	1000406-32-1	86
5	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80





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Operator : CG\JU
Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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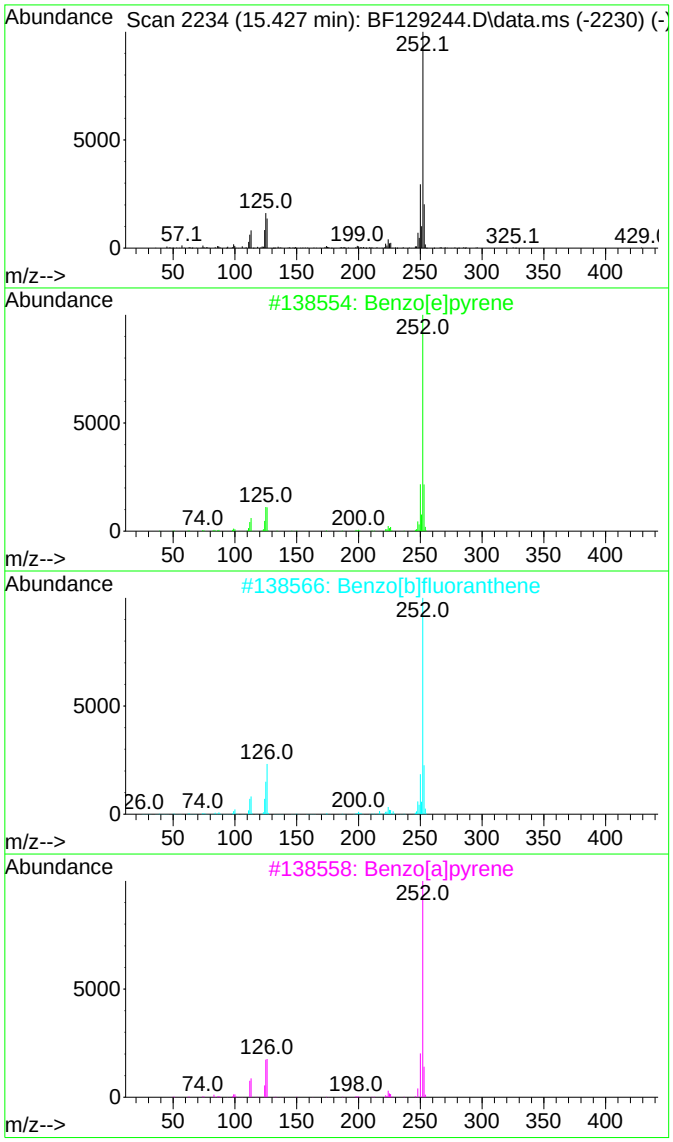
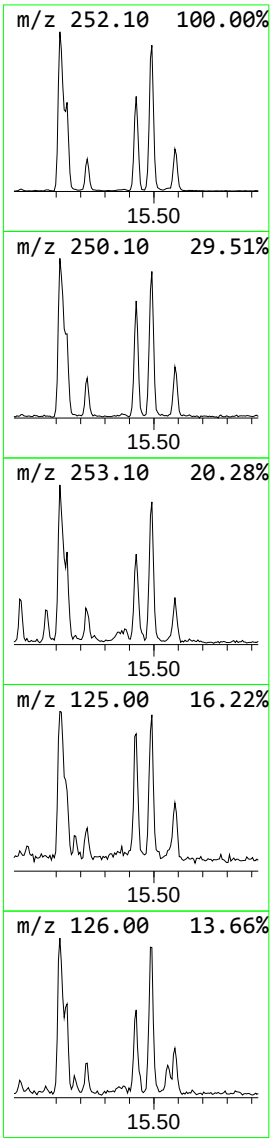
Peak Number 11 Benzo[e]pyrene Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.427	2.89 ng	232604	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzo[e]pyrene	252	C20H12	000192-97-2	97
2	Benzo[b]fluoranthene	252	C20H12	000205-99-2	94
3	Benzo[a]pyrene	252	C20H12	000050-32-8	93
4	Benzo[k]fluoranthene	252	C20H12	000207-08-9	93
5	Perylene	252	C20H12	000198-55-0	90





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Operator : CG\JU
Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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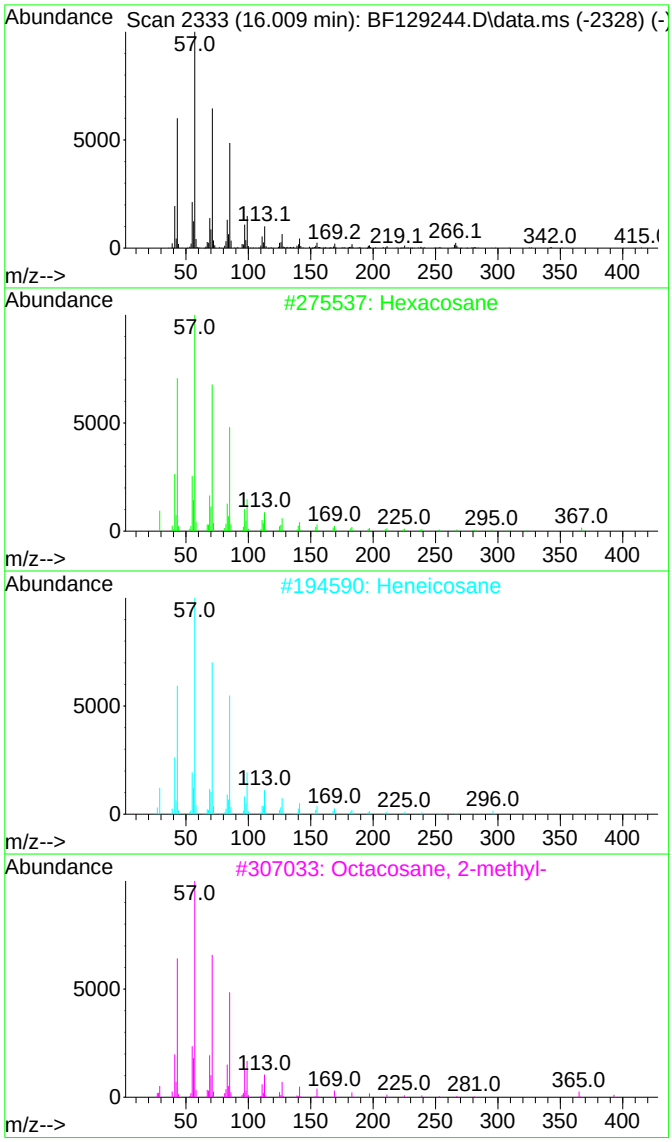
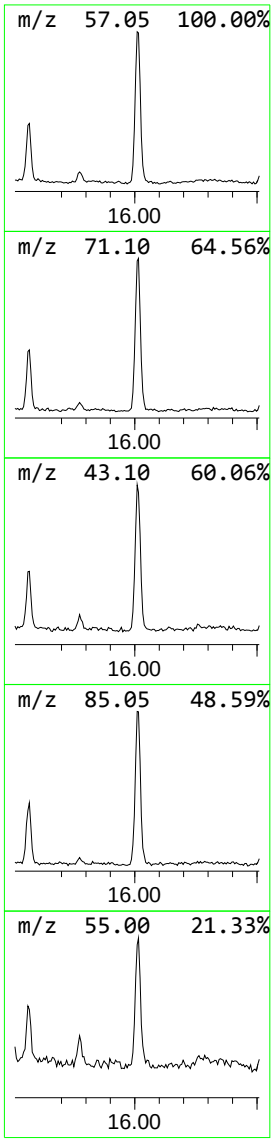
Peak Number 12 Heneicosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.009	6.66 ng	535713	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexacosane	366	C26H54	000630-01-3	94
2	Heneicosane	296	C21H44	000629-94-7	91
3	Octacosane, 2-methyl-	408	C29H60	001560-98-1	91
4	Docosane, 1-iodo-	436	C22H45I	1000406-31-9	87
5	Eicosane	282	C20H42	000112-95-8	87





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Operator : CG\JU
Sample : N3731-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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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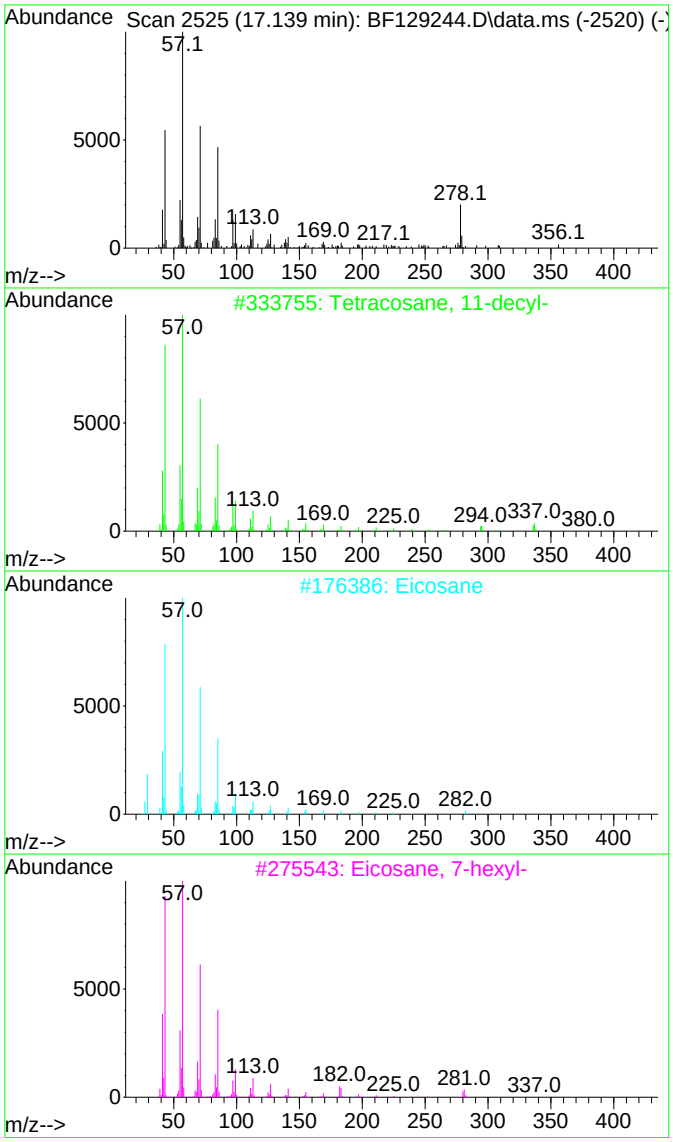
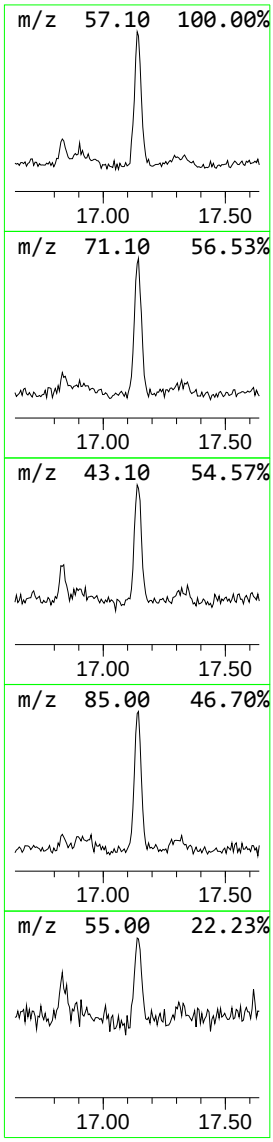
Peak Number 13 Tetracosane, 11-decyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.139	2.44 ng	196569	Perylene-d12	15.557

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane, 11-decyl-	479	C34H70	055429-84-0	68
2	Eicosane	282	C20H42	000112-95-8	68
3	Eicosane, 7-hexyl-	366	C26H54	055333-99-8	68
4	Octacosane, 2-methyl-	408	C29H60	001560-98-1	68
5	Hexacosane	366	C26H54	000630-01-3	68





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071522\
Data File : BF129244.D
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Operator : CG\JU
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Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF071522.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
Hexadecanoic ac...	11.810	2.8	ng	325343	4	11.427	2364140	20.0
n-Hexadecanoic ...	11.945	2.7	ng	316492	4	11.427	2364140	20.0
Heptadecane	13.574	2.3	ng	206747	5	14.068	1837760	20.0
Hexacosane	13.898	3.2	ng	296517	5	14.068	1837760	20.0
Triphenylphosph...	14.157	2.7	ng	250560	5	14.068	1837760	20.0
Heptacosane	14.216	3.6	ng	329734	5	14.068	1837760	20.0
Octacosane	14.521	3.9	ng	353344	5	14.068	1837760	20.0
Tetracosane	14.833	3.6	ng	288265	6	15.557	1608850	20.0
Hexacosanal	14.986	2.0	ng	161476	6	15.557	1608850	20.0
Octacosane, 1-i...	15.174	4.7	ng	377224	6	15.557	1608850	20.0
Benzo[e]pyrene	15.427	2.9	ng	232604	6	15.557	1608850	20.0
Heneicosane	16.009	6.7	ng	535713	6	15.557	1608850	20.0
Tetracosane, 11...	17.139	2.4	ng	196569	6	15.557	1608850	20.0