LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF127994.D
Acq On : 29 Apr 2022 14:55
Operator : CG\JU
Sample : N2602-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
12-15-SB4-BK-PRISON

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-BF042222.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127994.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.175	487	491	496	rVB	29836	38589	1.03%	0.138%
2	5.551	547	555	558	rBV	3027520	3101173	82.51%	11.076%
3	6.551	719	725	740	rVB	2882024	3237036	86.12%	11.562%
4	6.922	784	788	792	rVB	823817	655145	17.43%	2.340%
5	7.039	792	808	810	rBV3	38763	93540	2.49%	0.334%
6	7.486	879	884	887	rBV	2088542	2203403	58.62%	7.870%
7	8.204	1002	1006	1010	rBV	909171	836715	22.26%	2.988%
8	9.286	1184	1190	1193	rBV	3525834	3758691	100.00%	13.425%
9	9.551	1230	1235	1247	rBV	1951917	1993719	53.04%	7.121%
10	9.963	1300	1305	1309	rVB	1078028	999204	26.58%	3.569%
11	10.757	1434	1440	1443	rBV	2575564	2476125	65.88%	8.844%
12	11.457	1555	1559	1562	rBV	1219067	1014114	26.98%	3.622%
13	11.839	1615	1624	1626	rBV	83631	81298	2.16%	0.290%
14	11.969	1638	1646	1664	rBV	364173	585526	15.58%	2.091%
15	12.121	1669	1672	1678	rVB	61961	84282	2.24%	0.301%
16	12.245	1686	1693	1710	rBV	35777	166983	4.44%	0.596%
17	12.598	1749	1753	1760	rBV	423426	397810	10.58%	1.421%
18	12.680	1762	1767	1774	rVB5	29349	49408	1.31%	0.176%
19	12.757	1775	1780	1789	rVV	148500	171118	4.55%	0.611%
20	13.045	1824	1829	1833	rBV	3487345	3558594	94.68%	12.710%
21	13.198	1849	1855	1864	rBV3	35479	87580	2.33%	0.313%
22	13.963	1982	1985	1991	rVB2	52668	91861	2.44%	0.328%
23	14.063	1991	2002	2005	rBV6	73468	254276	6.77%	0.908%
24	14.104	2005	2009	2018	rVV	832559	773122	20.57%	2.761%
25	14.198	2018	2025	2031	rVV2	66331	86642	2.31%	0.309%
26	14.415	2059	2062	2066	rVB	94704	86722	2.31%	0.310%
27	14.557	2082	2086	2092	rBV	87358	118032	3.14%	0.422%
28	14.621	2093	2097	2102	rBV8	30100	47836	1.27%	0.171%
29	14.874	2137	2140	2145	rVB	44463	46244	1.23%	0.165%
30	15.139	2181	2185	2191	rBV4	37342	76081	2.02%	0.272%
31	15.227	2196	2200	2207	rVB	52533	71943	1.91%	0.257%
32	15.610	2260	2265	2274	rBV	477483	656640	17.47%	2.345%
33	15.804	2294	2298	2305	rVB4	21516	40417	1.08%	0.144%
34	16.080	2341	2345	2351	rVB2	39714	58344	1.55%	0.208%

Sum of corrected areas: 27998213

Instrument :
BNA_F
ClientSampleId :
12-15-SB4-BK-PRISON

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
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Acq On : 29 Apr 2022 14:55
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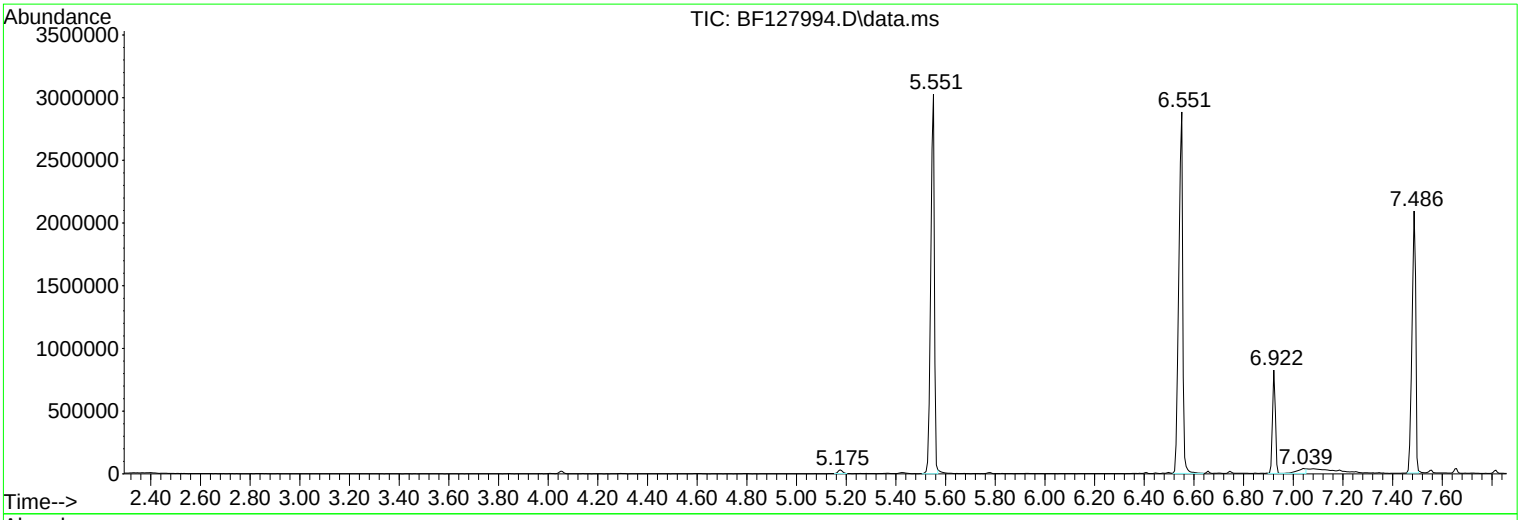
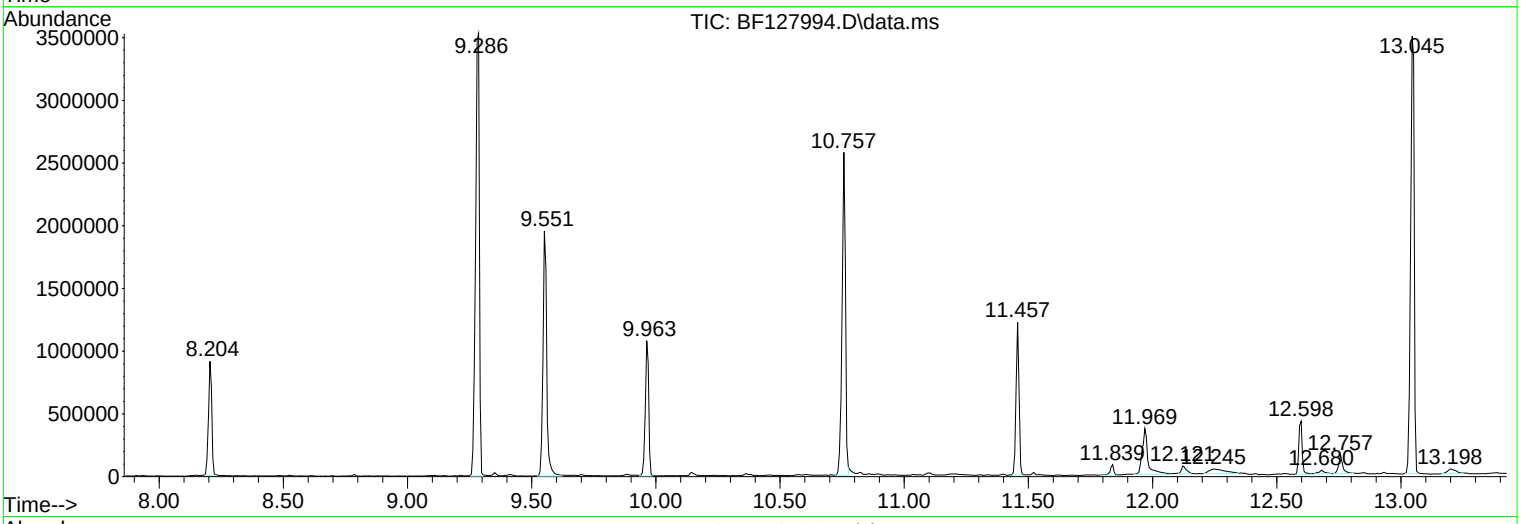
Misc :
ALS Vial : 5 Sample Multiplier: 1

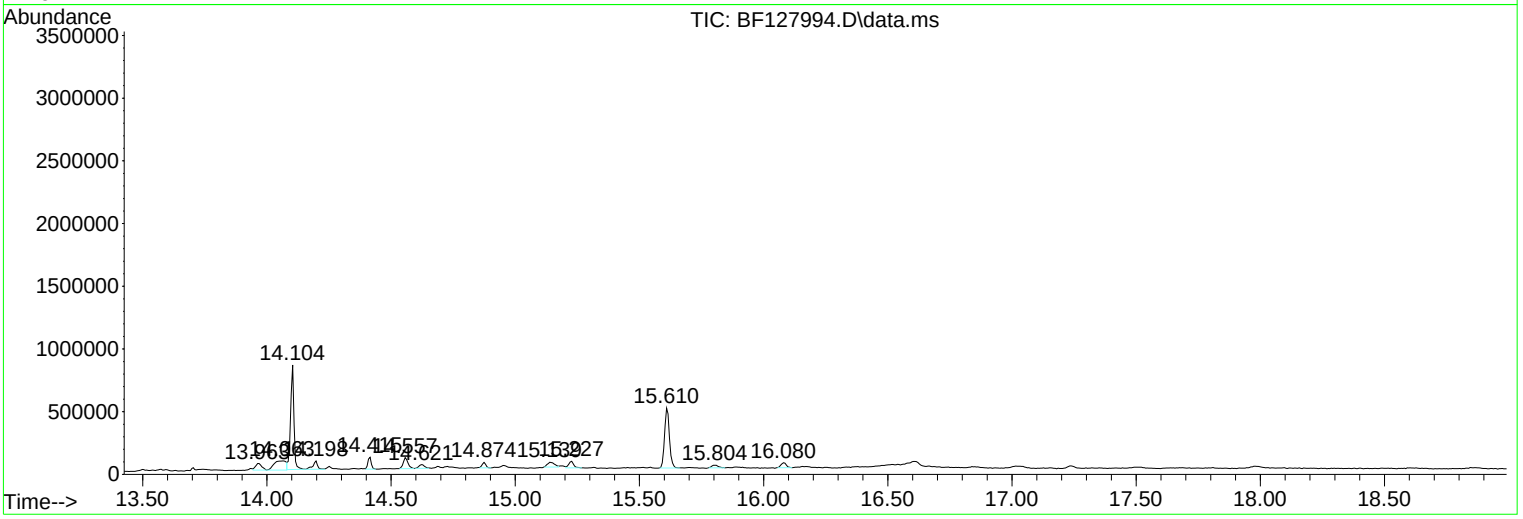
Instrument :
BNA_F
ClientSampleId :
12-15-SB4-BK-PRISON

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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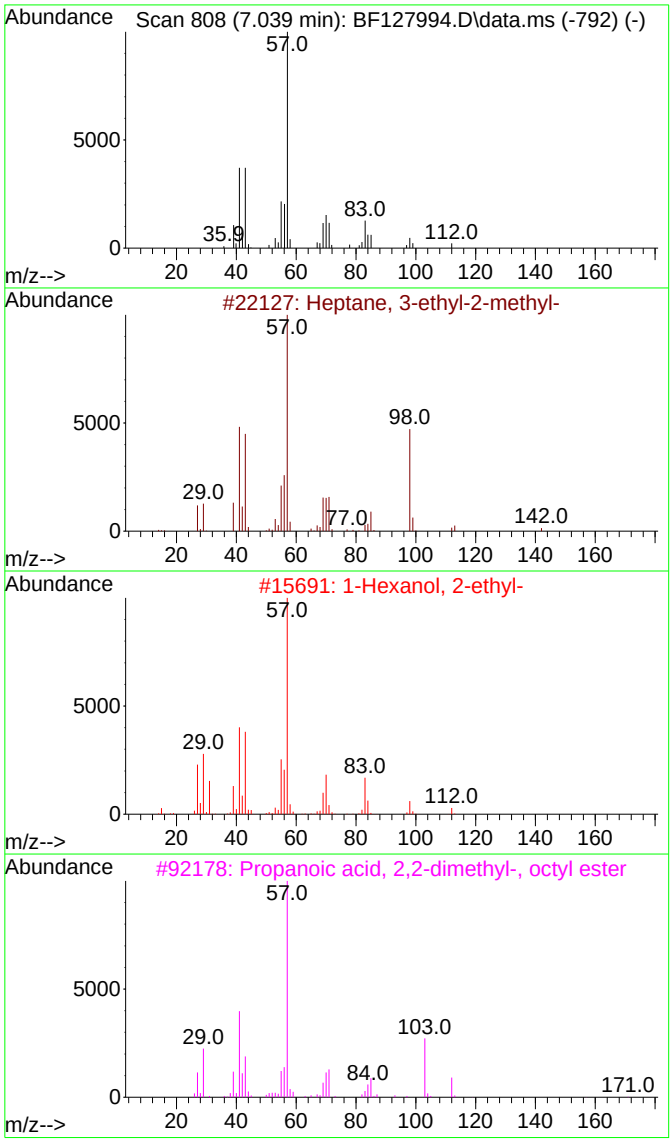
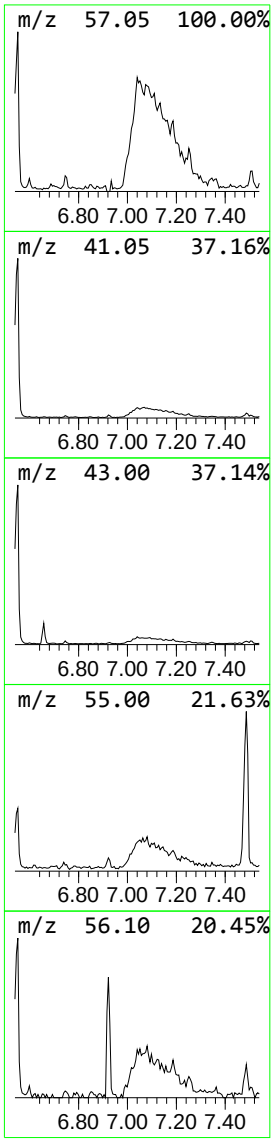
****
Peak Number 1 Heptane, 3-ethyl-2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.039	2.86 ng	93540	1,4-Dichlorobenzene-d4	6.922

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptane, 3-ethyl-2-methyl-	142	C10H22	014676-29-0	72
2	1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	72
3	Propanoic acid, 2,2-dimethyl-, o...	214	C13H26O2	027751-88-8	59
4	1-Hexene, 5,5-dimethyl-	112	C8H16	007116-86-1	59
5	Oxirane, [[(2-ethylhexyl)oxy]met...	186	C11H22O2	002461-15-6	56





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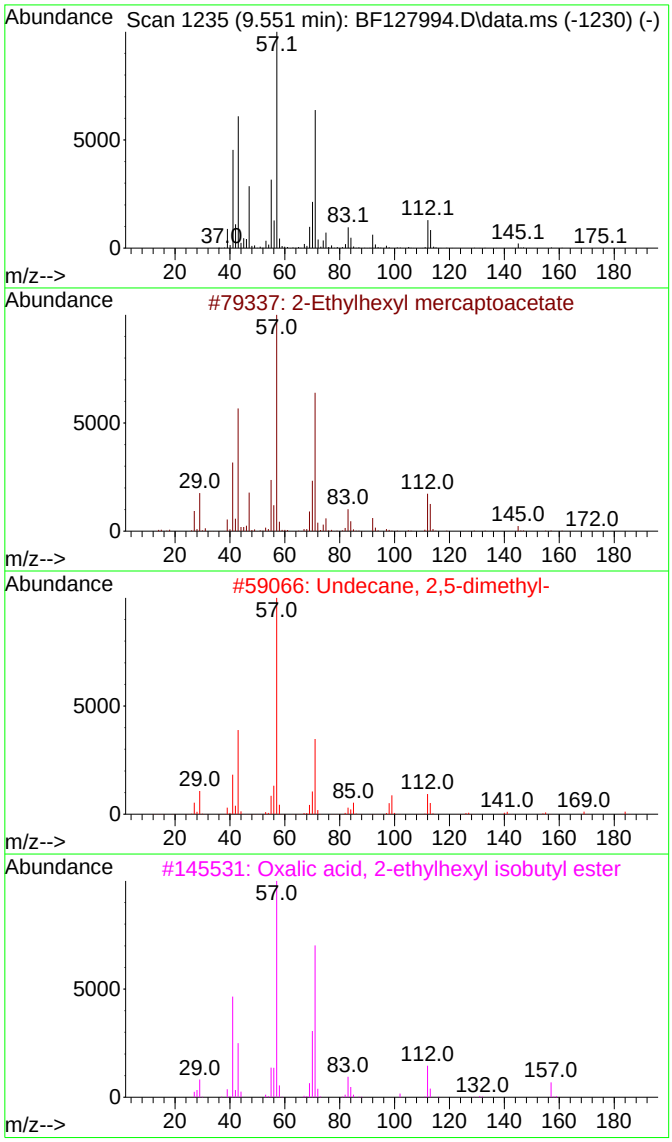
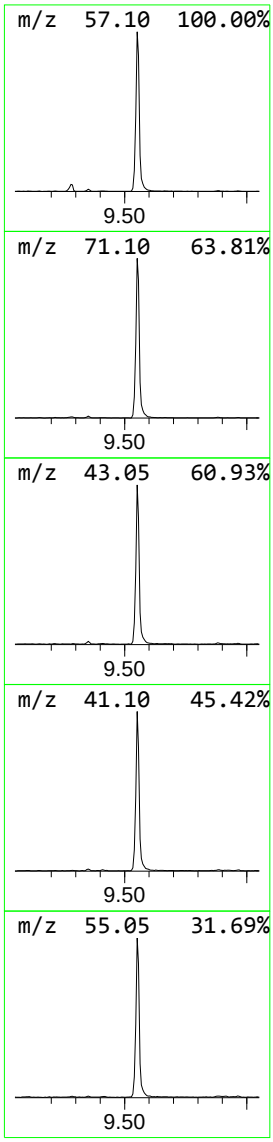
TIC Integration Parameters: LSCINT.P

****
Peak Number 2 2-Ethylhexyl mercaptoacetate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.551	39.91 ng	1993720	Acenaphthene-d10	9.963

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Ethylhexyl mercaptoacetate	204	C10H20O2S	007659-86-1	86
2	Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	64
3	Oxalic acid, 2-ethylhexyl isobut...	258	C14H26O4	1010309-38-5	50
4	Decane, 4-methyl-	156	C11H24	002847-72-5	50
5	Oxalic acid, bis(2-ethylhexyl) e...	314	C18H34O4	1000309-39-0	49





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TIC Library : C:\Database\NIST20.L
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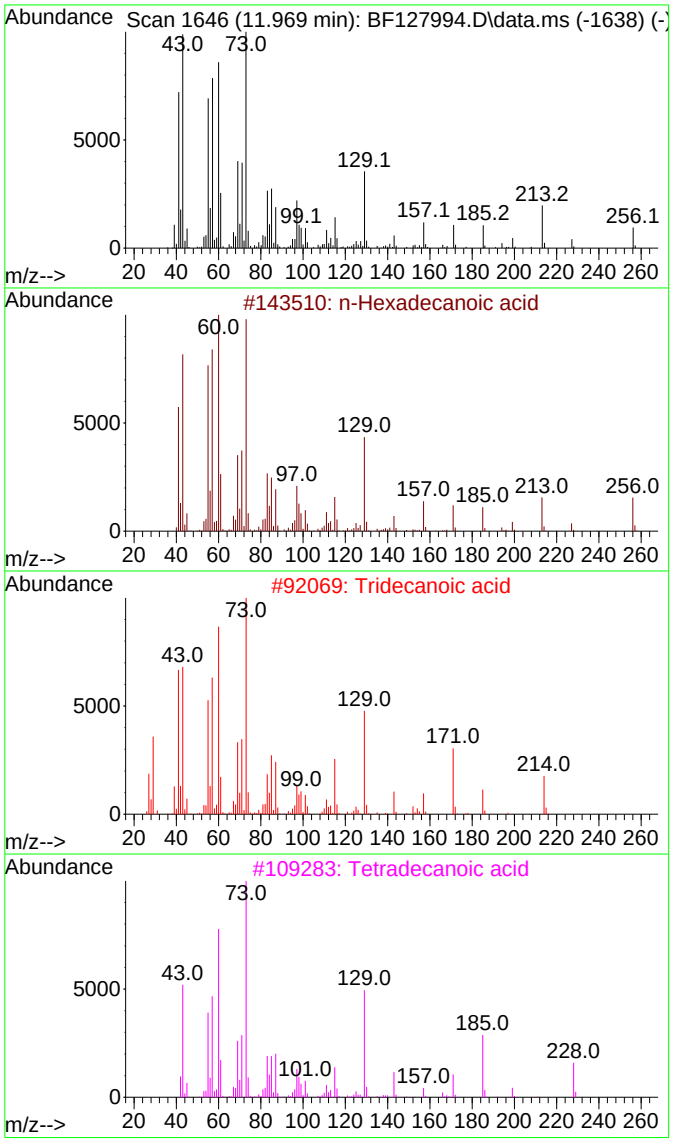
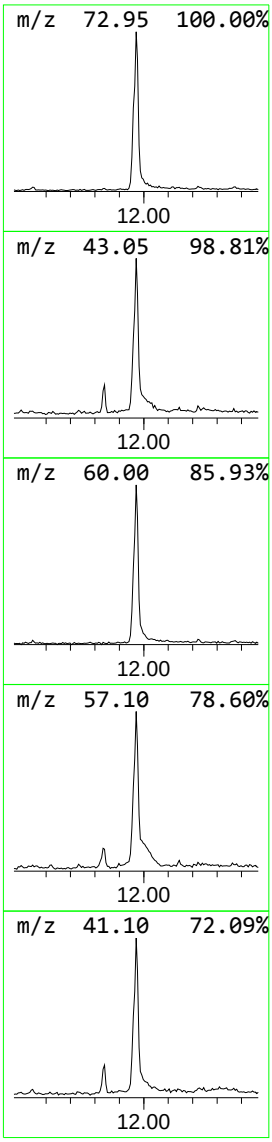
****

Peak Number 3 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.969	11.55 ng	585526	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
5	8-Methylnonanoic acid	172	C10H20O2	005963-14-4	46





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BNA_F
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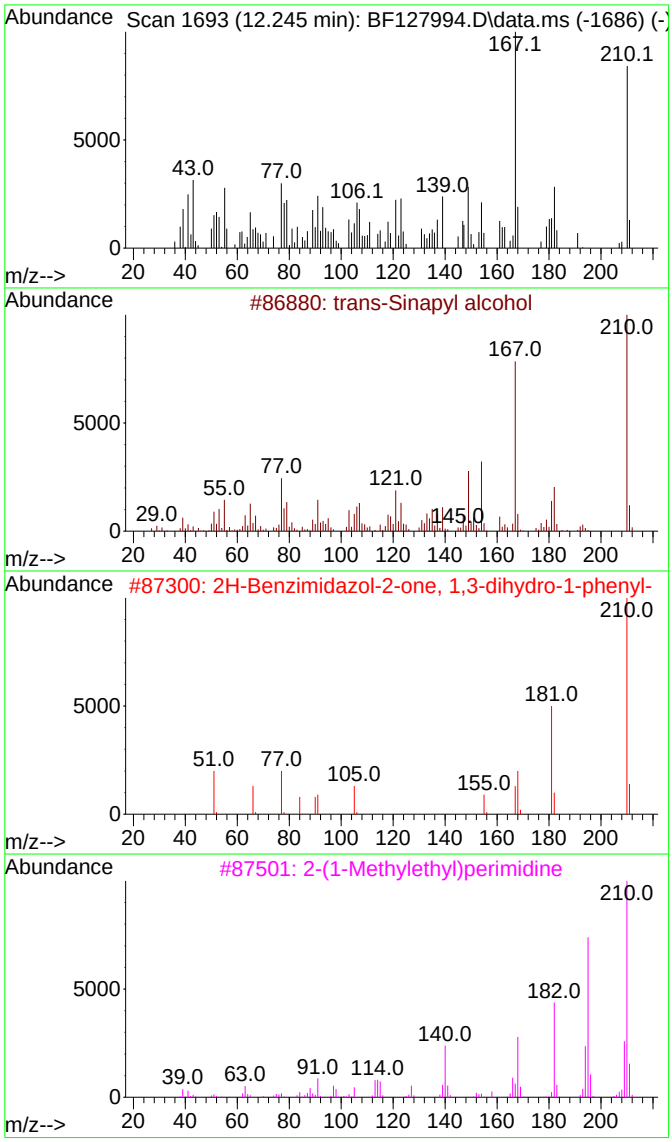
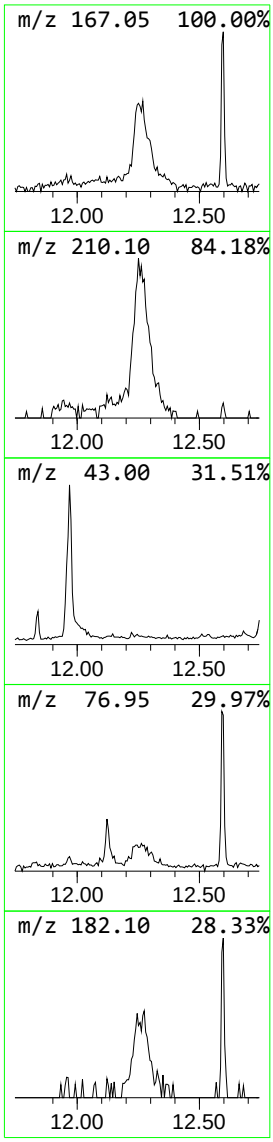
****

Peak Number 4 trans-Sinapyl alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.245	3.29 ng	166983	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	trans-Sinapyl alcohol	210	C11H14O4	020675-96-1	55
2	2H-Benzimidazol-2-one, 1,3-dihyd...	210	C13H10N2O	014813-85-5	30
3	2-(1-Methylethyl)perimidine	210	C14H14N2	028478-14-0	30
4	1,4-benzenediamine, N4,N4-diethy...	182	C10H15FN2	1000404-88-0	25
5	Benzenemethanol, 2,5-dimethoxy-,...	210	C11H14O4	067698-75-3	25





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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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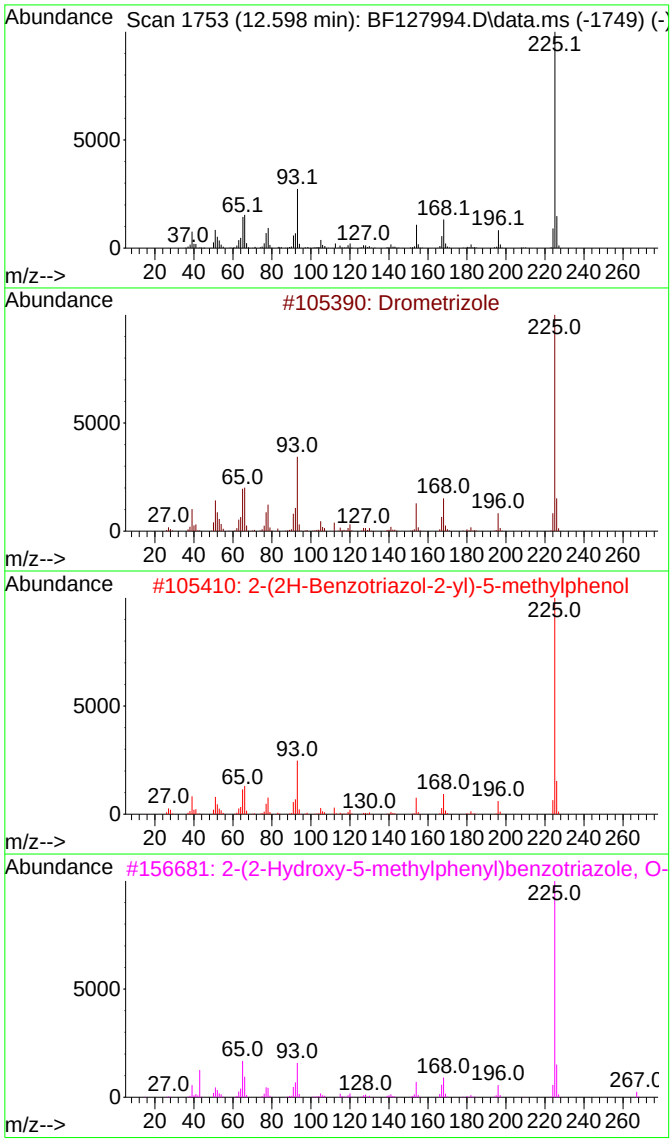
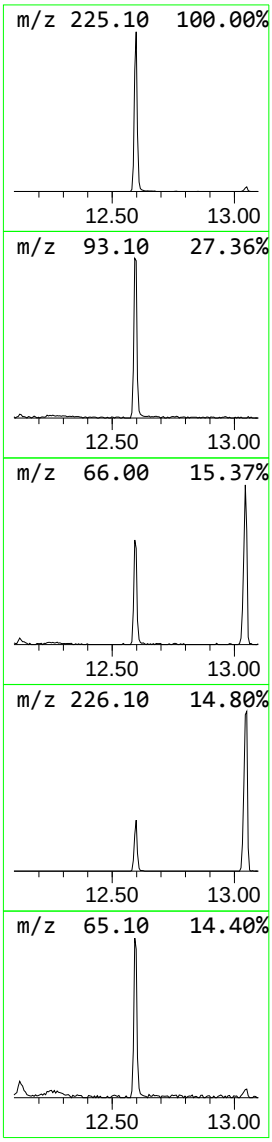
****

Peak Number 5 Drometrizole Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.598	7.85 ng	397810	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Drometrizole	225	C13H11N3O	002440-22-4	97
2	2-(2H-Benzotriazol-2-yl)-5-methy...	225	C13H11N3O	004998-48-5	97
3	2-(2-Hydroxy-5-methylphenyl)benz...	267	C15H13N3O2	1000384-15-2	86
4	6-Aminobenzo(g)quinoxaline-5,10-...	225	C12H7N3O2	072225-24-2	49
5	4-Amino-2-oxo-1,2-dihydro[1]benz...	225	C12H7N3O2	078993-57-4	47





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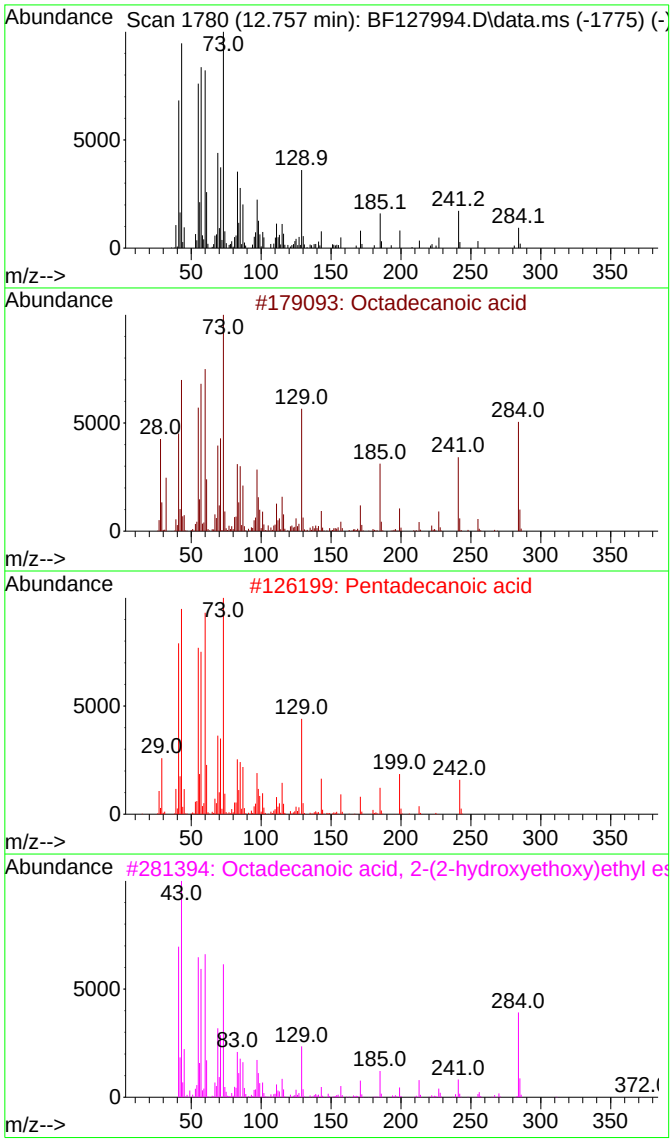
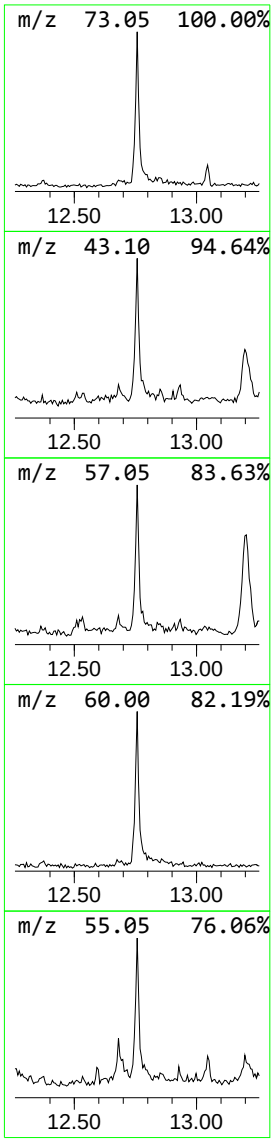
****

Peak Number 6 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.757	3.37 ng	171118	Phenanthrene-d10	11.457

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
3	Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5	Dodecanoic acid	200	C12H24O2	000143-07-7	59





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

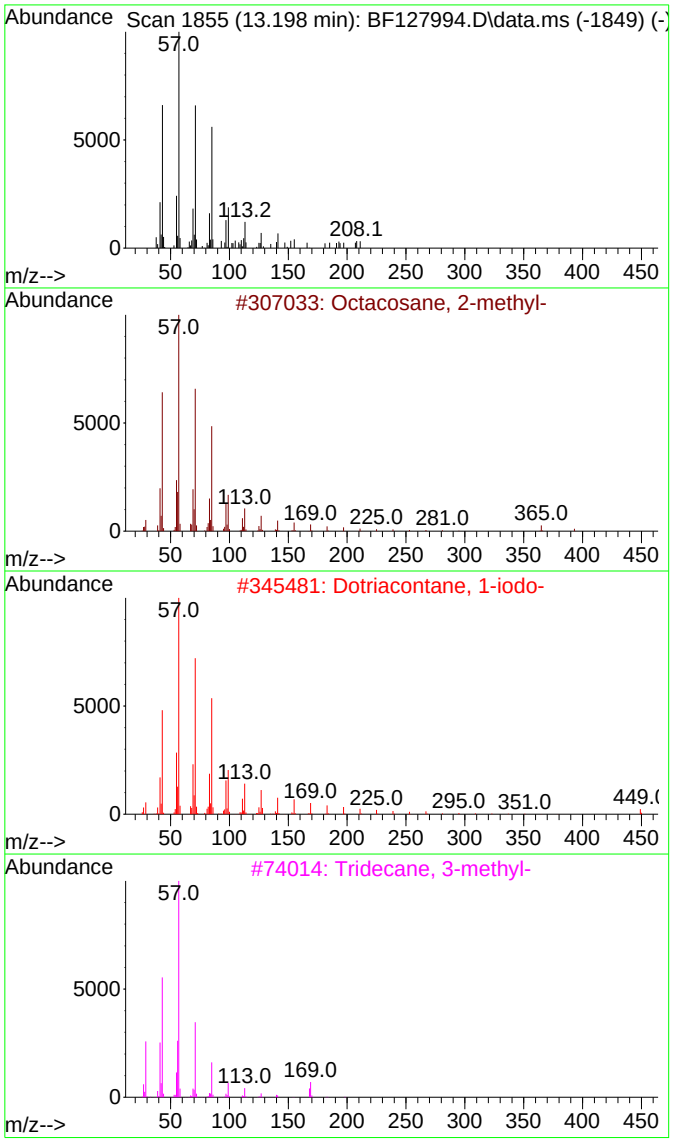
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

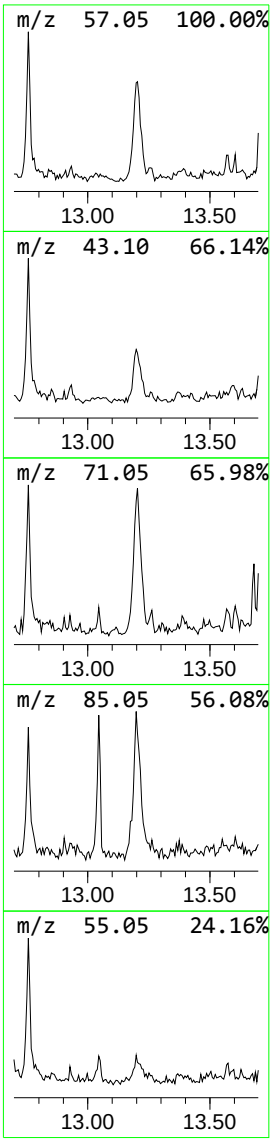
****

Peak Number 7 Octacosane, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.198	2.27 ng	87580	Chrysene-d12	14.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosane, 2-methyl-	408	C29H60	001560-98-1	90
2	Dotriacontane, 1-iodo-	576	C32H65I	1000406-32-4	83
3	Tridecane, 3-methyl-	198	C14H30	006418-41-3	80
4	Hexadecane	226	C16H34	000544-76-3	78
5	Heptacosane	380	C27H56	000593-49-7	78





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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
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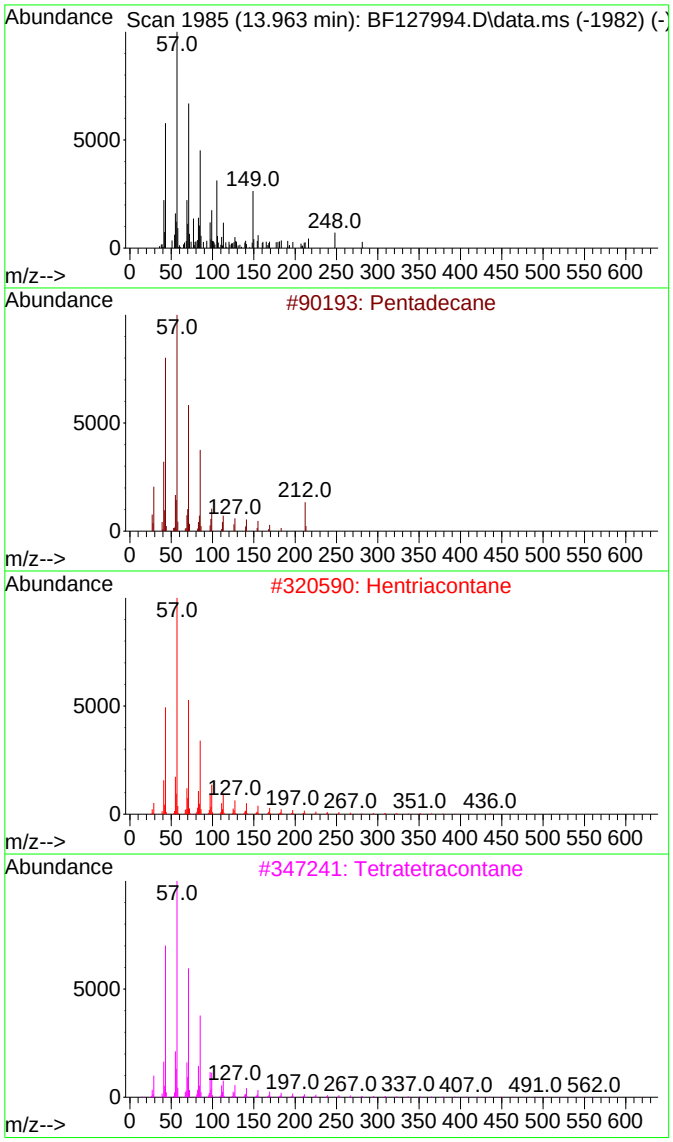
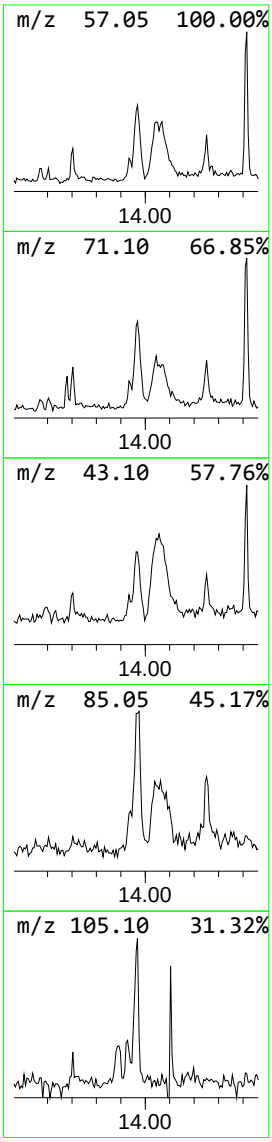
Peak Number 8 Pentadecane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.963	2.38 ng	91861	Chrysene-d12	14.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane	212	C15H32	000629-62-9	64
2	Hentriacontane	437	C31H64	000630-04-6	62
3	Tetratetracontane	619	C44H90	007098-22-8	62
4	Heptacosane	380	C27H56	000593-49-7	62
5	Pentacosane	352	C25H52	000629-99-2	58





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ALS Vial : 5 Sample Multiplier: 1

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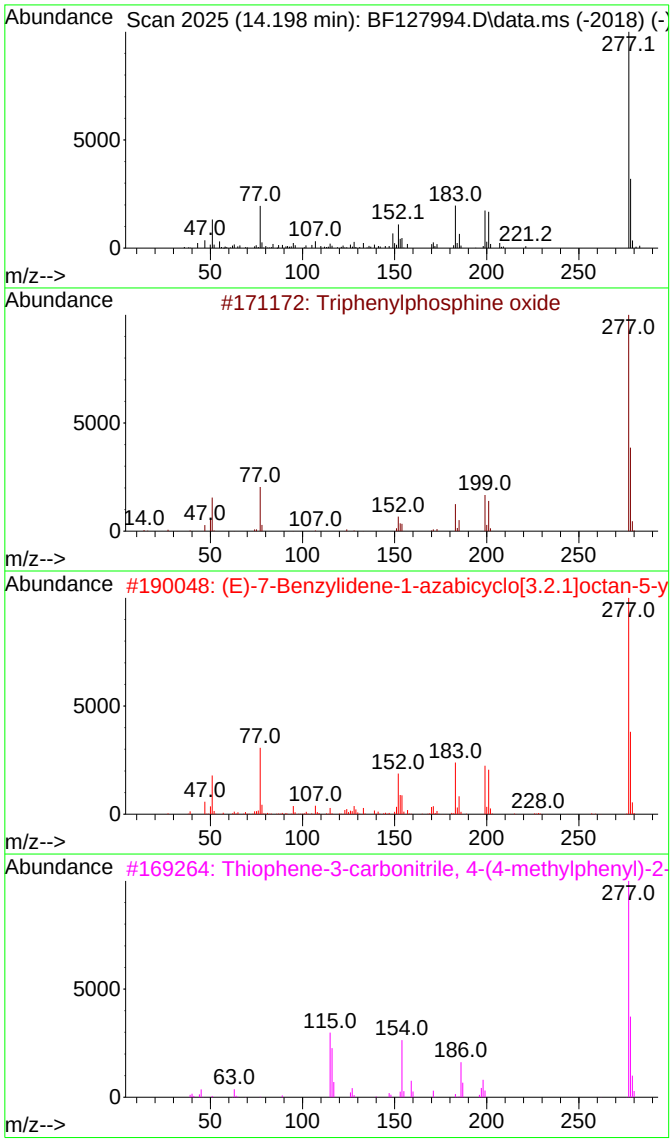
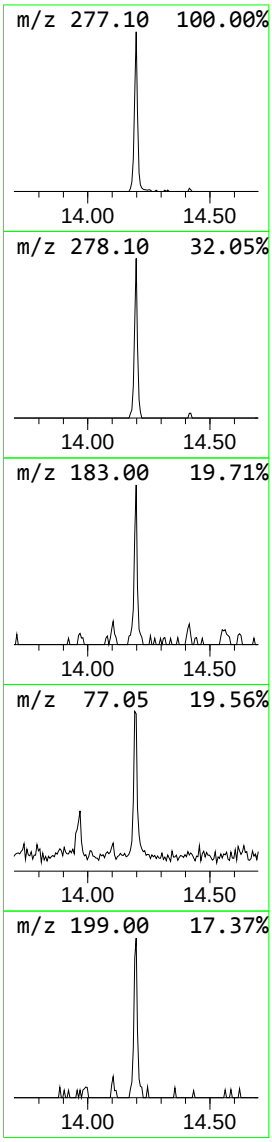
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 9 Triphenylphosphine oxide Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.198	2.24 ng	86642	Chrysene-d12	14.104

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	50
3	Thiophene-3-carbonitrile, 4-(4-m...	277	C13H11NO2S2	1000268-75-0	37
4	5-Methyl-8-phenylfuro[3',2':5,6]...	277	C16H11N3O2	1000460-07-9	33
5	3-(3,4-Dichlorophenyl)-2-thioxo-...	277	C9H5Cl2NOS2	017046-34-3	32





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF127994.D
Acq On : 29 Apr 2022 14:55
Operator : CG\JU
Sample : N2602-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
12-15-SB4-BK-PRISON

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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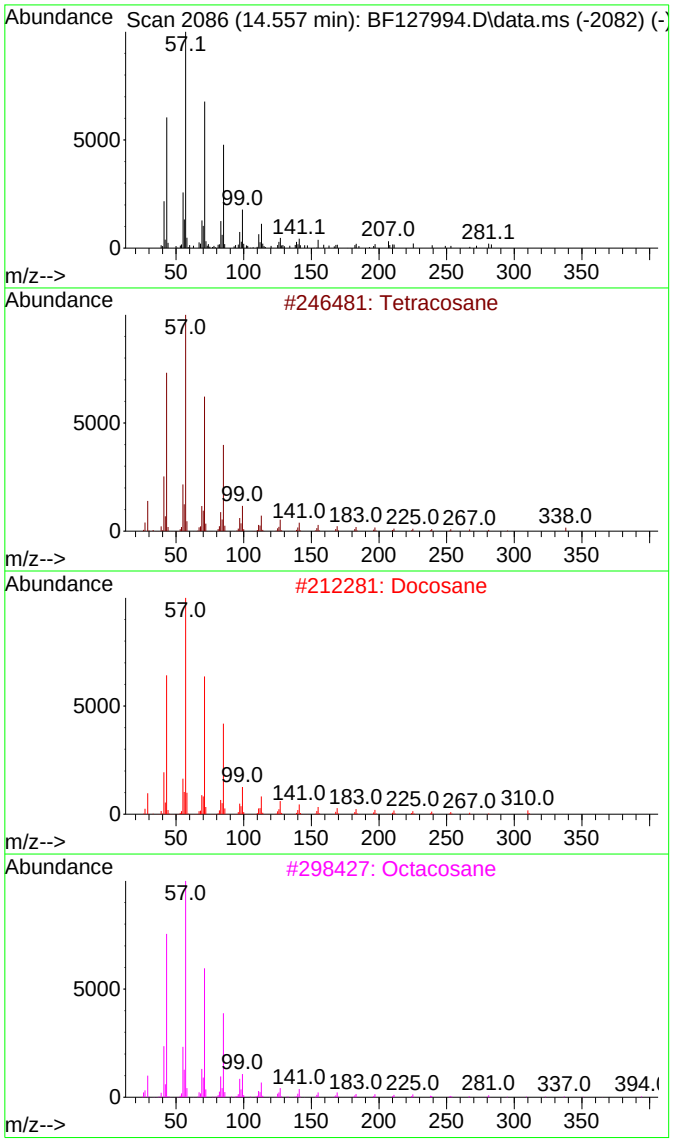
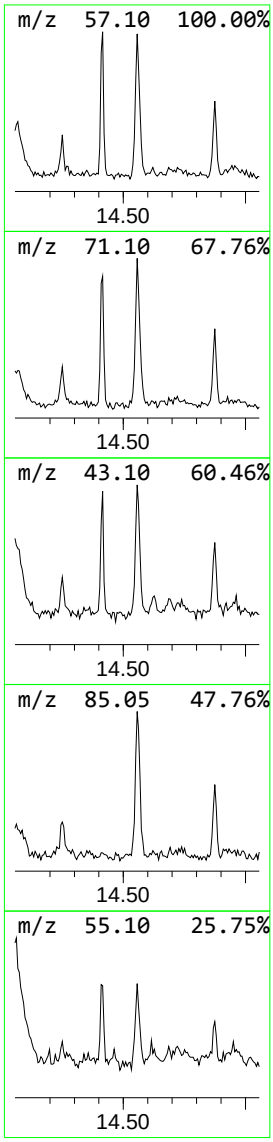
Peak Number 11 Tetracosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.557	3.05 ng	118032	Chrysene-d12	14.104

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tetracosane	338	C24H50	000646-31-1	90
2	Docosane	310	C22H46	000629-97-0	87
3	Octacosane	394	C28H58	000630-02-4	87
4	Triacontane	422	C30H62	000638-68-6	87
5	Eicosane	282	C20H42	000112-95-8	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF127994.D
Acq On : 29 Apr 2022 14:55
Operator : CG\JU
Sample : N2602-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
12-15-SB4-BK-PRISON

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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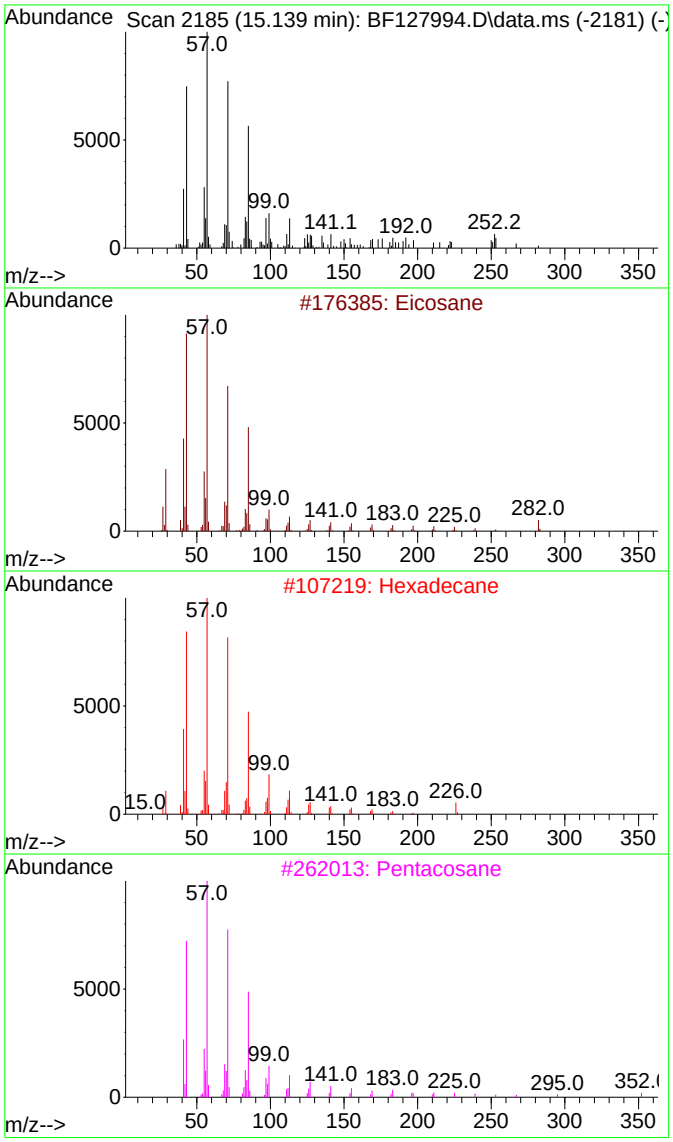
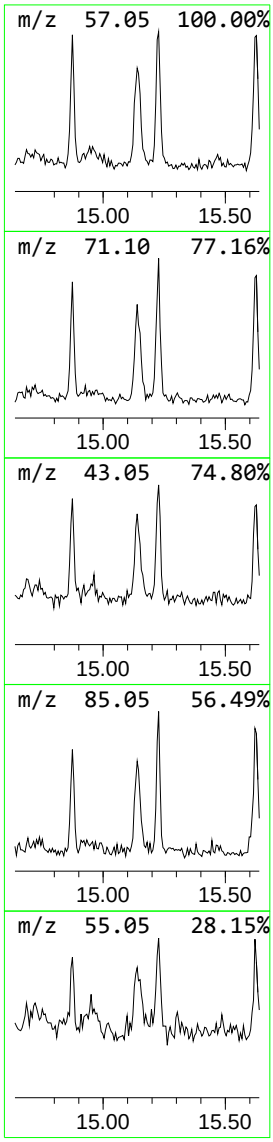
Peak Number 12 Eicosane Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.139	2.32 ng	76081	Perylene-d12	15.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	87
2	Hexadecane	226	C16H34	000544-76-3	86
3	Pentacosane	352	C25H52	000629-99-2	86
4	Heneicosane, 11-(1-ethylpropyl)-	366	C26H54	055282-11-6	86
5	Triacontane	422	C30H62	000638-68-6	86





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF127994.D
Acq On : 29 Apr 2022 14:55
Operator : CG\JU
Sample : N2602-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
12-15-SB4-BK-PRISON

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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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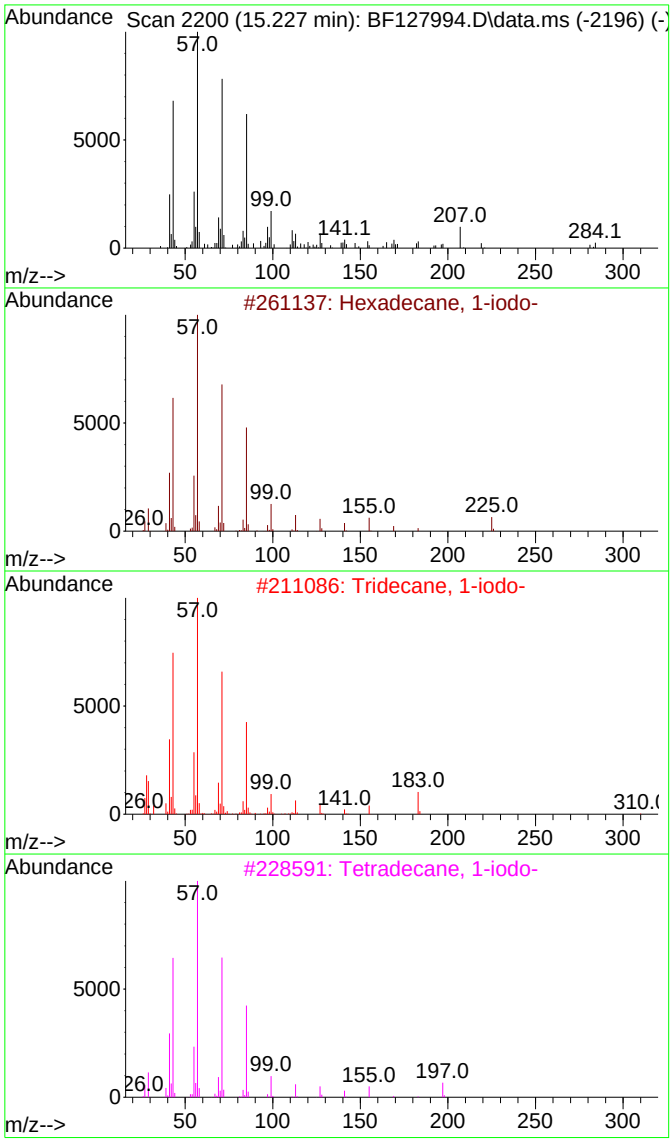
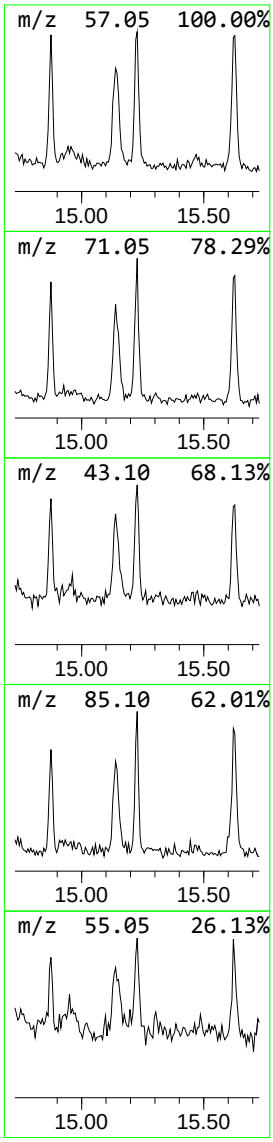
Peak Number 13 Hexadecane, 1-iodo- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.227	2.19 ng	71943	Perylene-d12	15.610

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	80
2	Tridecane, 1-iodo-	310	C13H27I	035599-77-0	80
3	Tetradecane, 1-iodo-	324	C14H29I	019218-94-1	80
4	Octadecane, 1-iodo-	380	C18H37I	000629-93-6	80
5	Hexacosane	366	C26H54	000630-01-3	72





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF042922\
Data File : BF127994.D
Acq On : 29 Apr 2022 14:55
Operator : CG\JU
Sample : N2602-03
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
12-15-SB4-BK-PRISON

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF042222.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
Heptane, 3-ethy...	7.039	2.9	ng	93540	1	6.922	655145	20.0
2-Ethylhexyl me...	9.551	39.9	ng	1993720	3	9.963	999204	20.0
n-Hexadecanoic ...	11.969	11.6	ng	585526	4	11.457	1014110	20.0
trans-Sinapyl a...	12.245	3.3	ng	166983	4	11.457	1014110	20.0
Drometrizole	12.598	7.8	ng	397810	4	11.457	1014110	20.0
Octadecanoic acid	12.757	3.4	ng	171118	4	11.457	1014110	20.0
Octacosane, 2-m...	13.198	2.3	ng	87580	5	14.104	773122	20.0
Pentadecane	13.963	2.4	ng	91861	5	14.104	773122	20.0
Triphenylphosph...	14.198	2.2	ng	86642	5	14.104	773122	20.0
Tetracosane	14.557	3.0	ng	118032	5	14.104	773122	20.0
Eicosane	15.139	2.3	ng	76081	6	15.610	656640	20.0
Hexadecane, 1-i...	15.227	2.2	ng	71943	6	15.610	656640	20.0