

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
 Data File : BF123588.D
 Acq On : 16 Apr 2021 12:43
 Operator : JU/CG
 Sample : M2048-09
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-03-14.5-15.0

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-BF041521.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123588.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.146	3	10	16	rVB	2927480	3801871	49.85%	6.916%
2	5.487	573	578	581	rBV	7211495	6870006	90.08%	12.497%
3	6.493	744	749	753	rBV	6030255	7159608	93.88%	13.023%
4	6.863	809	812	816	rBV	1471294	1263349	16.57%	2.298%
5	7.428	903	908	911	rBV	4508879	4678627	61.35%	8.510%
6	8.151	1027	1031	1034	rBV	2052519	1611849	21.14%	2.932%
7	9.234	1209	1215	1218	rBV	8484634	7070346	92.71%	12.861%
8	9.622	1278	1281	1285	rBV	256590	204960	2.69%	0.373%
9	9.910	1326	1330	1334	rBV	2136540	1739515	22.81%	3.164%
10	10.704	1460	1465	1468	rBV	5850764	5257862	68.94%	9.564%
11	11.398	1580	1583	1587	rBV	2040115	1890732	24.79%	3.439%
12	11.933	1671	1674	1684	rBV	448690	406539	5.33%	0.739%
13	12.875	1830	1834	1842	rBV	501046	627082	8.22%	1.141%
14	12.998	1850	1855	1858	rVB	8078167	7626266	100.00%	13.872%
15	13.686	1969	1972	1977	rVB2	159336	143265	1.88%	0.261%
16	13.904	2005	2009	2021	rVB	627085	1081911	14.19%	1.968%
17	14.045	2030	2033	2041	rVB	1560338	1527842	20.03%	2.779%
18	14.216	2059	2062	2065	rBV	91767	88388	1.16%	0.161%
19	14.339	2080	2083	2087	rVB	109108	89996	1.18%	0.164%
20	14.521	2111	2114	2116	rBV	114649	116784	1.53%	0.212%
21	14.551	2116	2119	2129	rVB6	90008	186104	2.44%	0.339%
22	15.186	2223	2227	2233	rVB	105235	120497	1.58%	0.219%
23	15.533	2281	2286	2291	rBV	959326	1164564	15.27%	2.118%
24	16.027	2365	2370	2377	rVB2	61558	93771	1.23%	0.171%
25	17.680	2645	2651	2657	rBV10	52935	153557	2.01%	0.279%

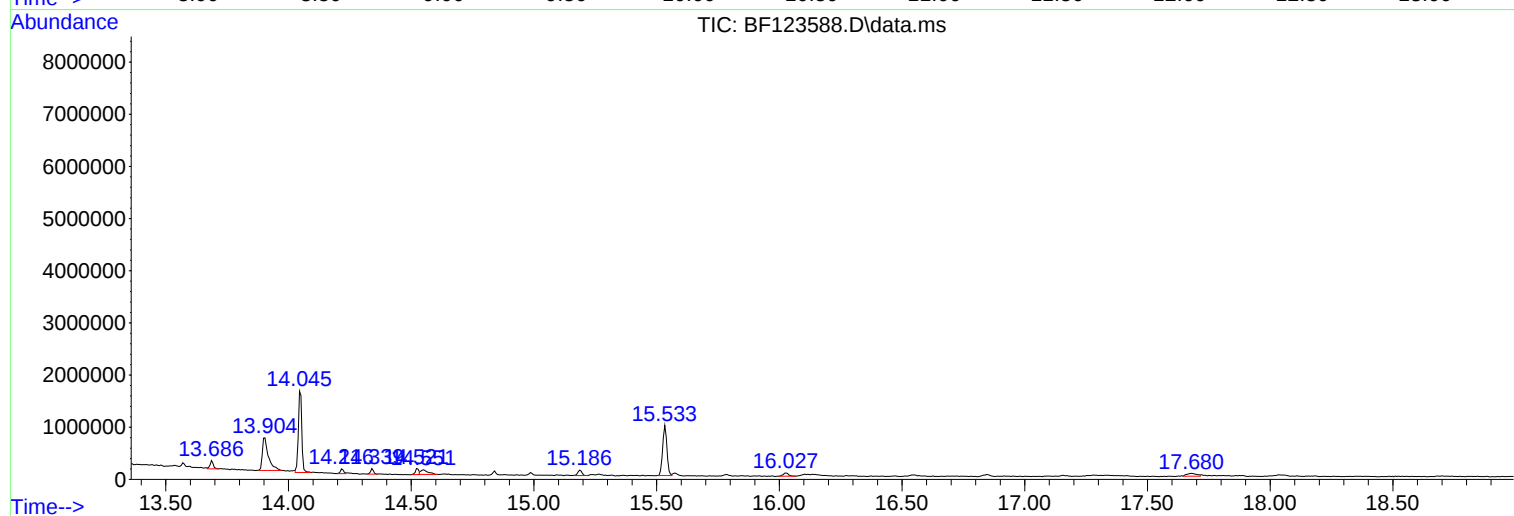
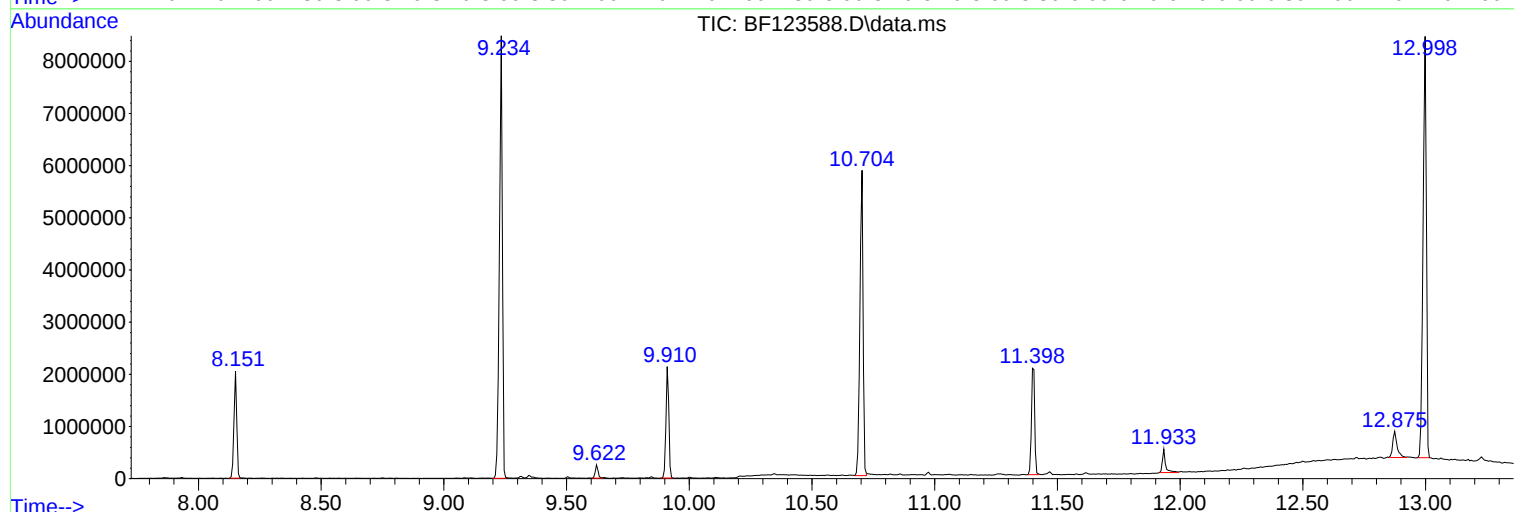
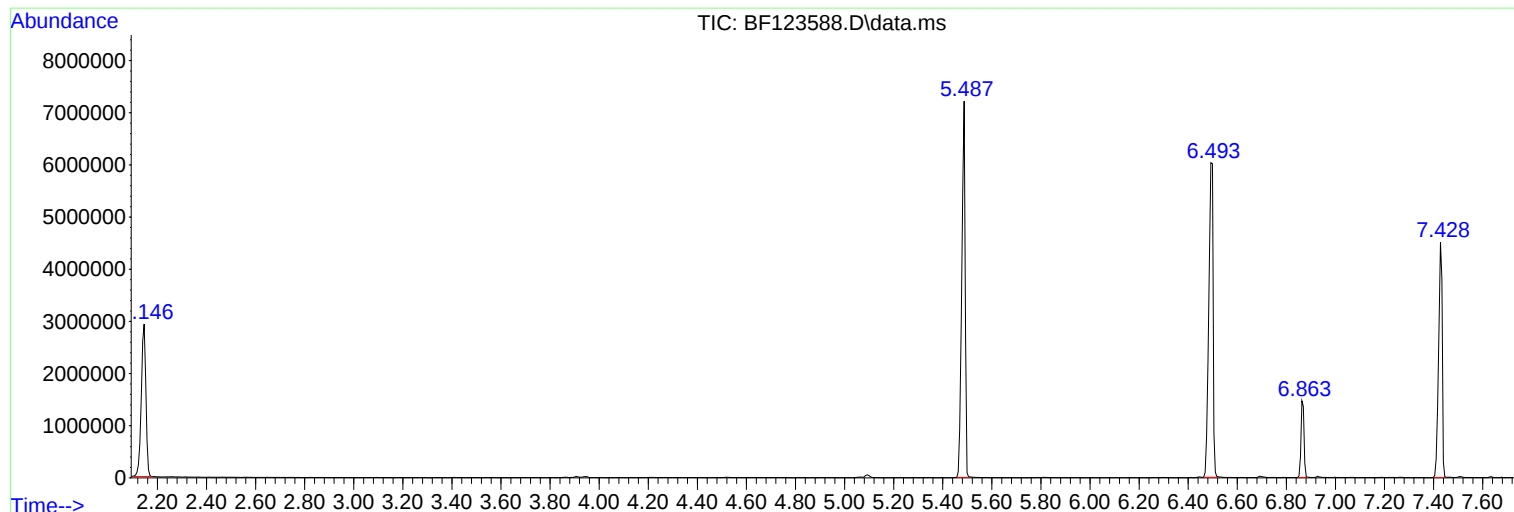
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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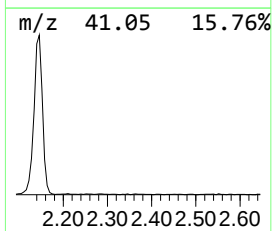
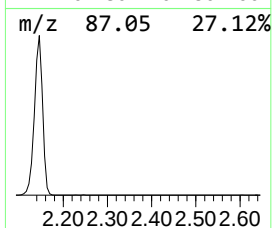
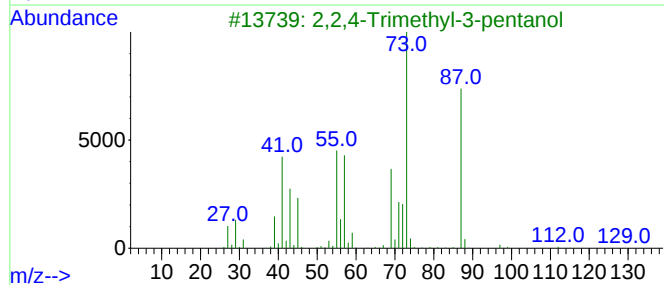
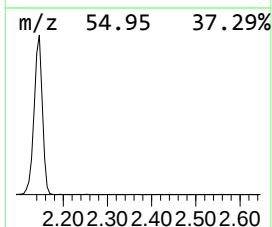
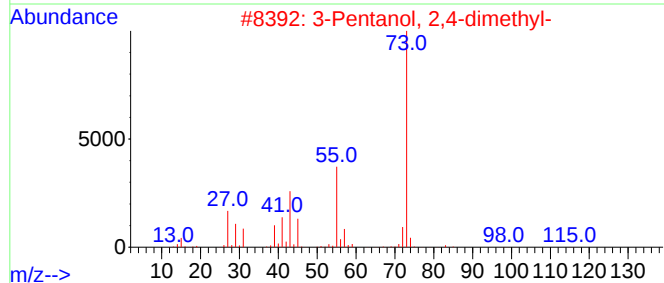
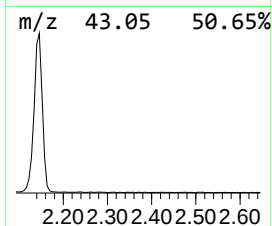
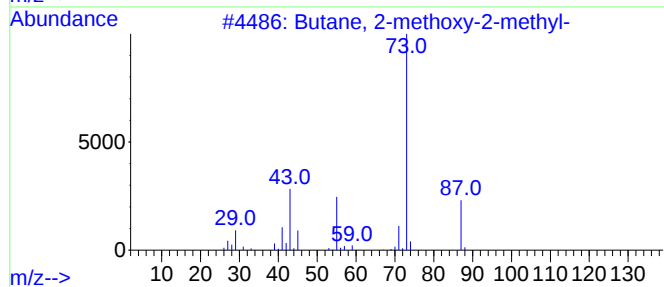
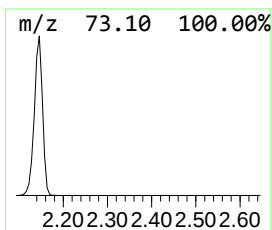
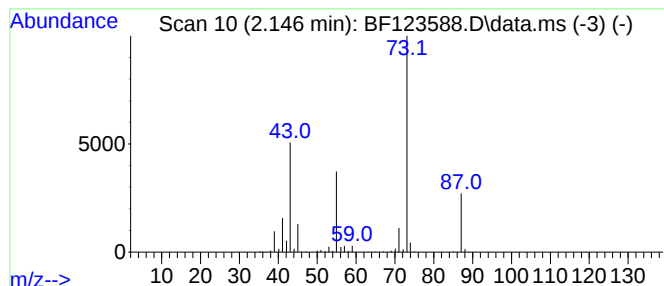
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.146	60.19 ng	3801870	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	83
2			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	43
3			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
4			Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
5			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23



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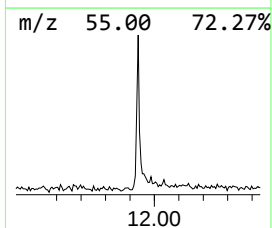
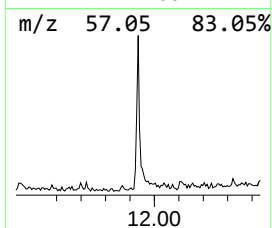
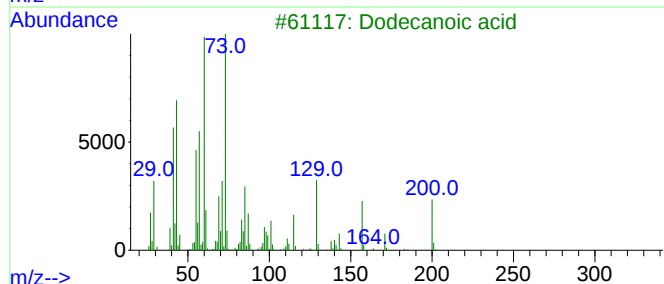
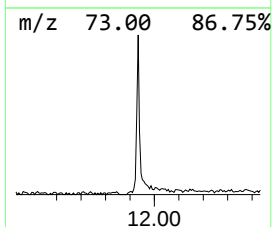
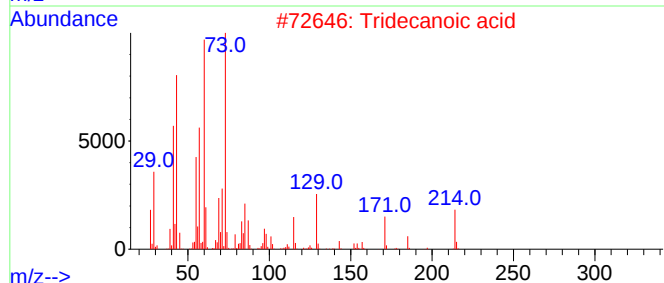
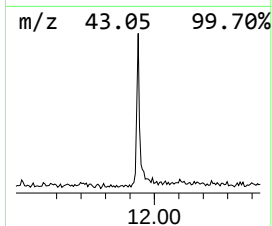
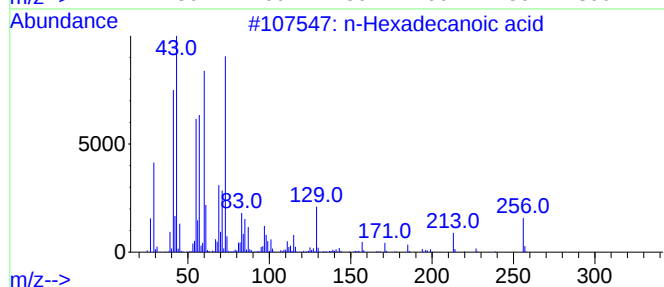
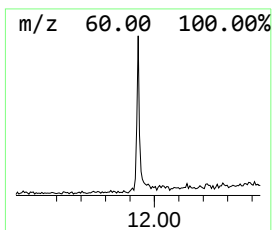
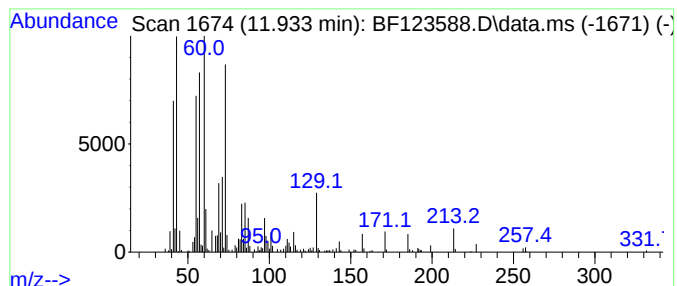
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.933	4.30 ng	406539	Phenanthrene-d10	11.404

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	90
2			Tridecanoic acid	214	C13H26O2	000638-53-9	86
3			Dodecanoic acid	200	C12H24O2	000143-07-7	80
4			Undecanoic acid	186	C11H22O2	000112-37-8	64
5			Tetradecanoic acid	228	C14H28O2	000544-63-8	64



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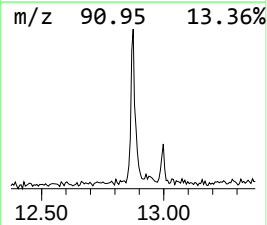
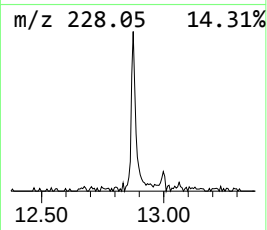
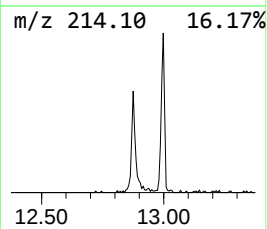
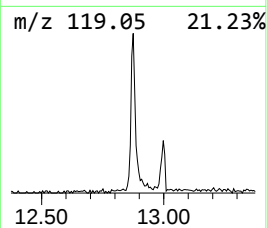
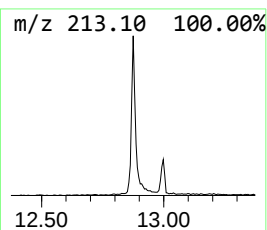
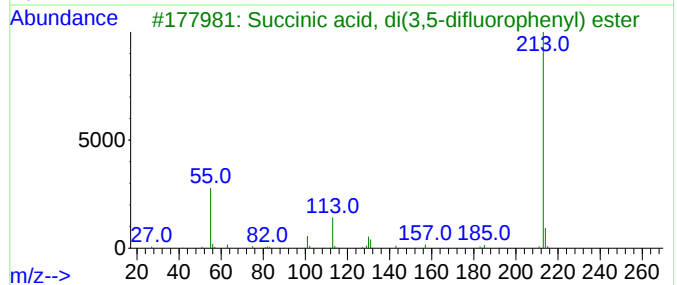
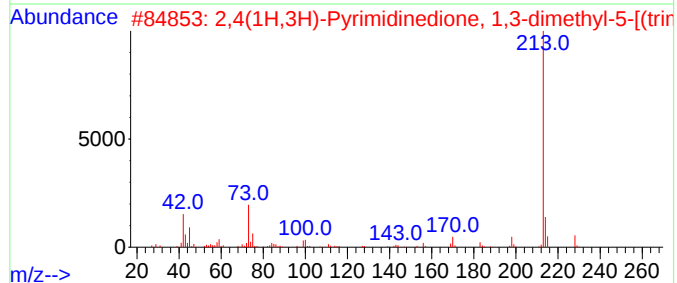
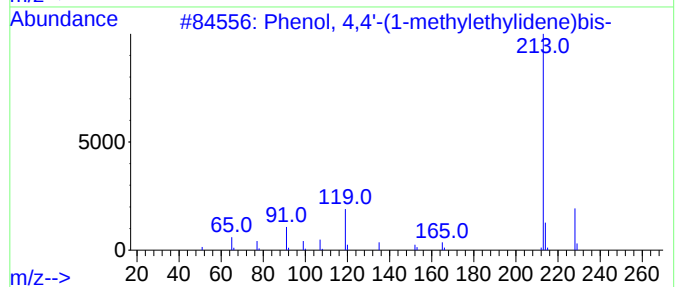
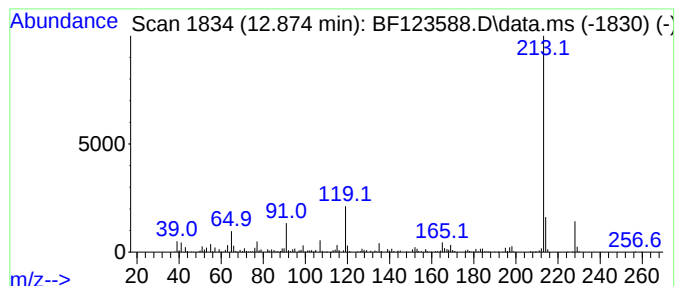
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Phenol, 4,4'-(1-methylethyl... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.874	8.21 ng	627082	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	95
2			2,4(1H,3H)-Pyrimidinedione, 1,3-...	228	C9H16N2O3Si	089447-84-7	53
3			Succinic acid, di(3,5-difluoroph...	342	C16H10F4O4	1000358-04-1	50
4			Decanedioic acid, diethyl ester	258	C14H26O4	000110-40-7	50
5			Carbanilic acid, p-phenyl-	213	C13H11NO2	004474-53-7	50



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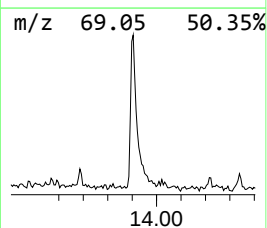
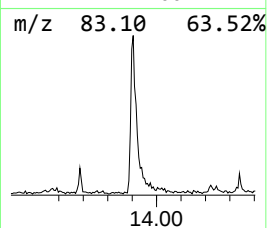
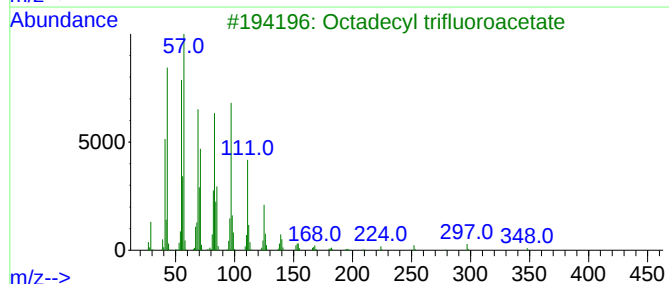
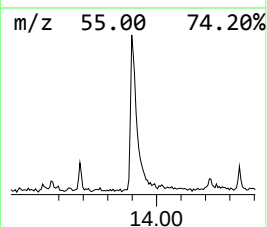
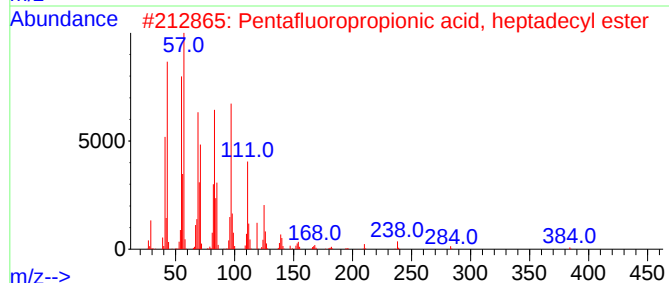
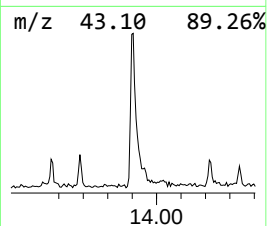
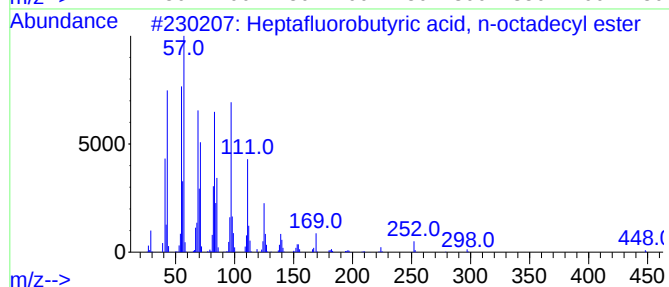
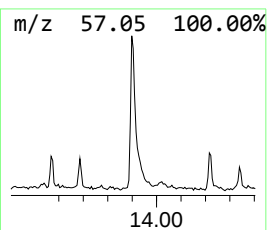
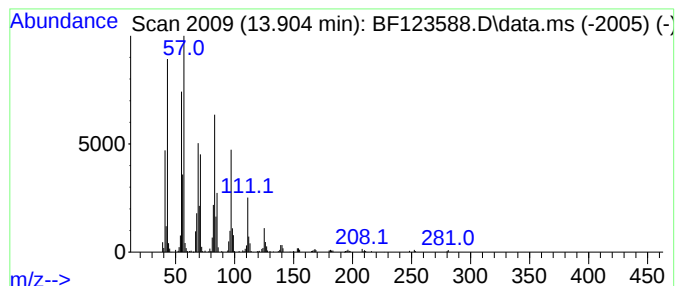
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Peak Number 4 Heptafluorobutyric acid, n-... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	14.16 ng	1081910	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	91
2			Pentafluoropropionic acid, heptadecyl ester	402	C20H35F5O2	959218-78-1	91
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4			Heptafluorobutyric acid, hexadecyl ester	438	C20H33F7O2	006385-15-5	91
5			Eicosyl pentafluoropropionate	444	C23H41F5O2	1000351-80-8	91



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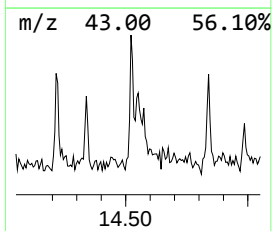
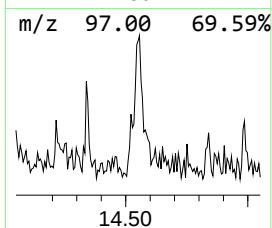
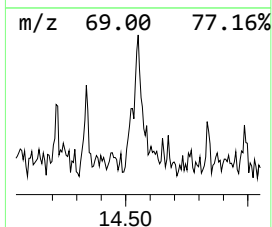
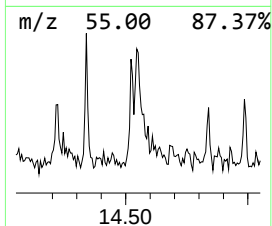
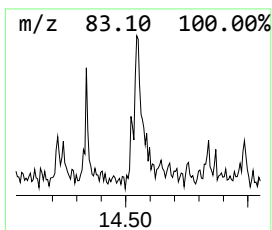
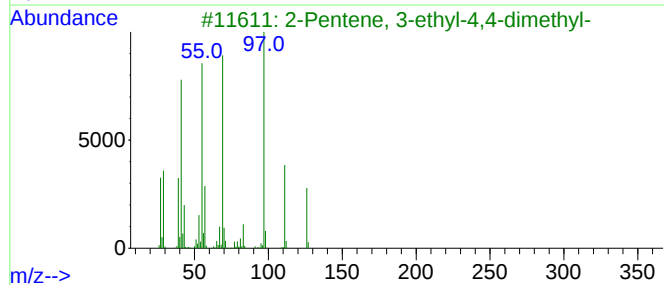
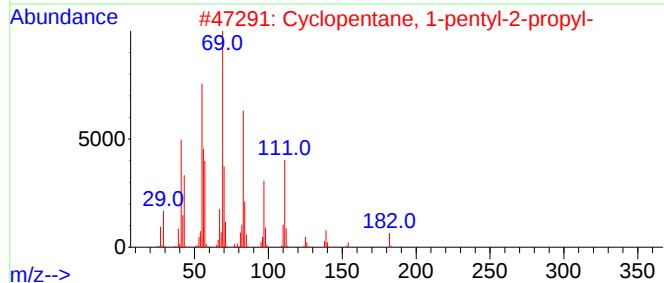
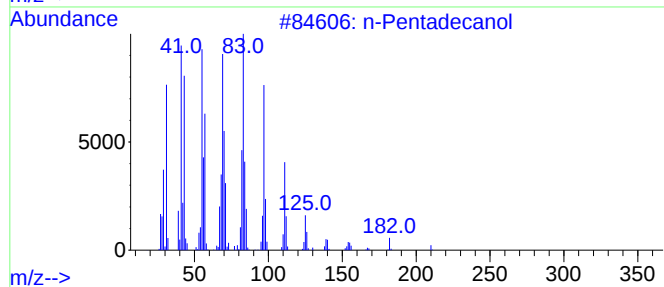
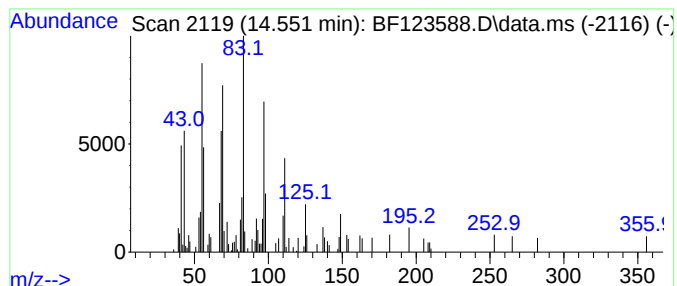
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Pentadecanol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.551	2.44 ng	186104	Chrysene-d12	14.045

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Pentadecanol	228	C15H32O	000629-76-5	78
2			Cyclopentane, 1-pentyl-2-propyl-	182	C13H26	062199-51-3	47
3			2-Pentene, 3-ethyl-4,4-dimethyl-	126	C9H18	053907-59-8	27
4			Cyclopentanone, 3-methyl-	98	C6H10O	001757-42-2	27
5			3-Hexene, 2-methyl-, (Z)-	98	C7H14	015840-60-5	25



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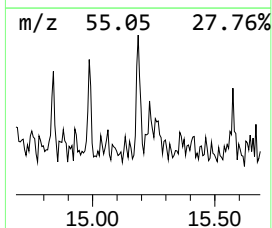
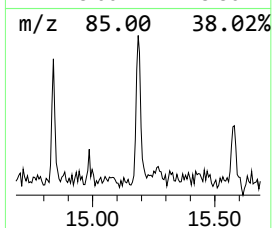
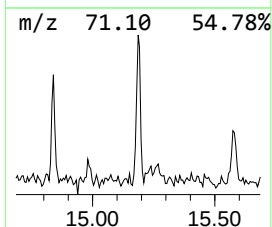
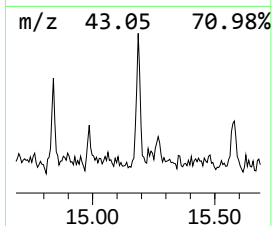
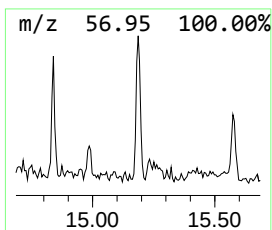
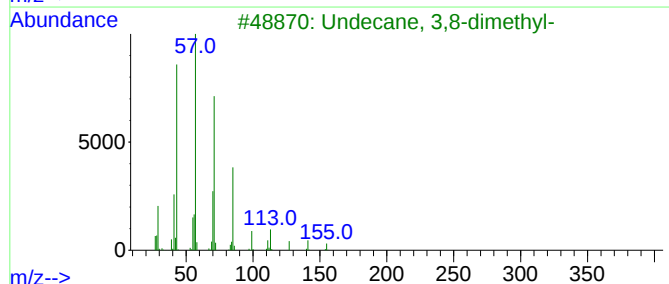
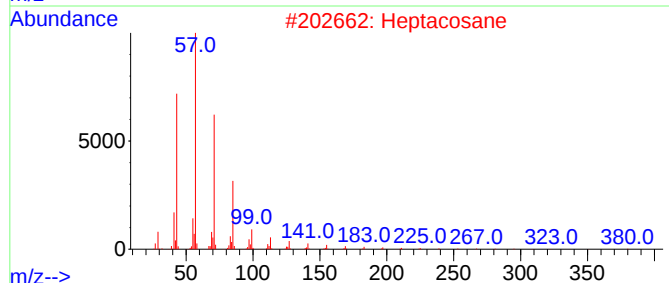
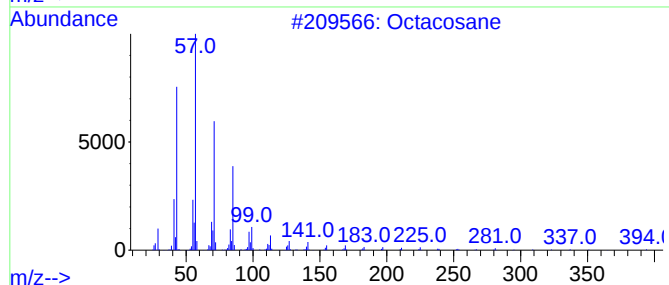
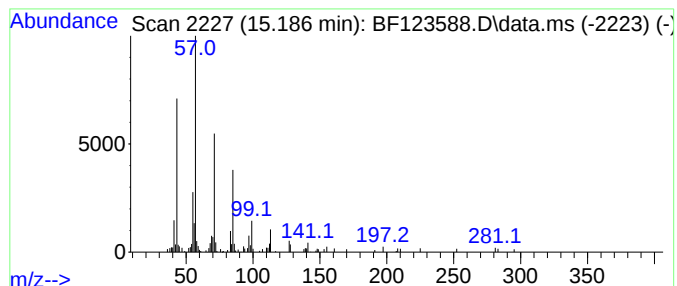
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Octacosane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.186	2.07 ng	120497	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octacosane	394	C28H58	000630-02-4	83
2			Heptacosane	380	C27H56	000593-49-7	80
3			Undecane, 3,8-dimethyl-	184	C13H28	017301-30-3	80
4			Hexatriacontane	507	C36H74	000630-06-8	80
5			2-Bromotetradecane	276	C14H29Br	074036-95-6	80



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123588.D
Acq On : 16 Apr 2021 12:43
Operator : JU/CG
Sample : M2048-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-14.5-15.0

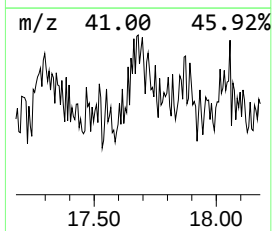
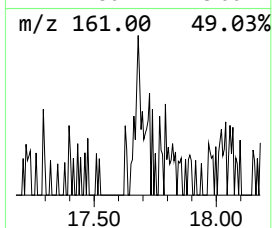
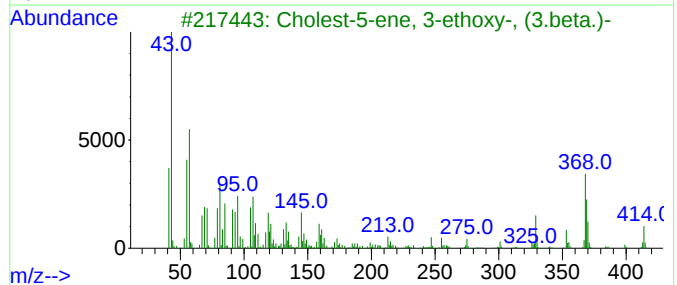
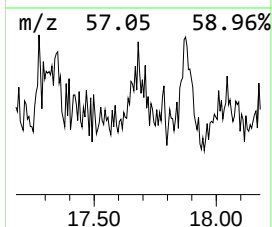
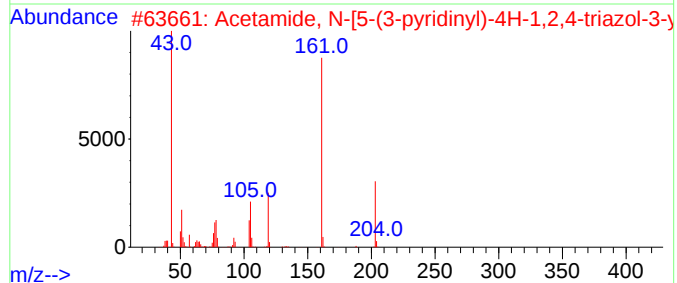
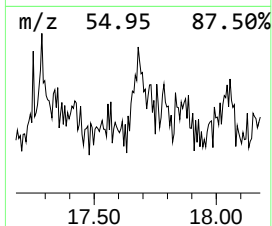
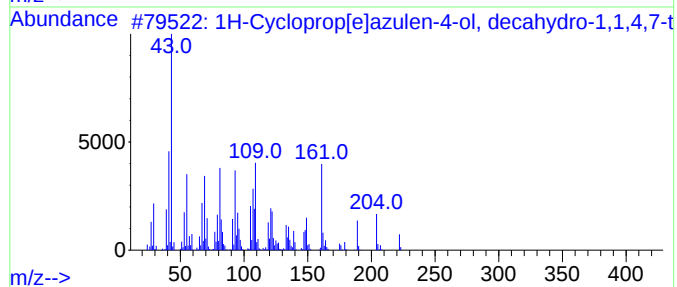
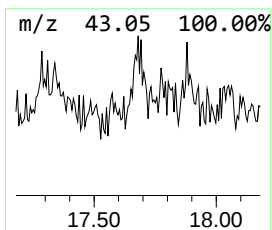
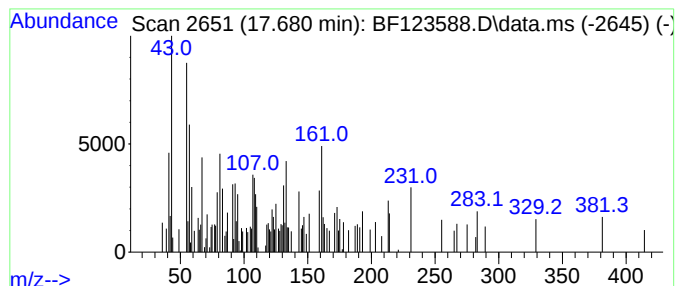
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown17.680 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.680	2.64 ng	153557	Perylene-d12	15.533

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Cycloprop[e]azulen-4-ol, deca...	222	C15H26O	000552-02-3	10
2			Acetamide, N-[5-(3-pyridinyl)-4H...	203	C9H9N5O	1000337-51-5	10
3			Cholest-5-ene, 3-ethoxy-, (3.bet...	414	C29H50O	000986-19-6	10
4			5-Amino-2-methyl-2-(2-oxopropyl)...	230	C11H10N4O2	1000326-97-3	9
5			Ethanone, 1-(1,2,3,4,7,7a-hexahy...	246	C17H26O	032388-58-2	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF041621\
Data File : BF123588.D
Acq On : 16 Apr 2021 12:43
Operator : JU/CG
Sample : M2048-09
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-03-14.5-15.0

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF041521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.146	60.2	ng	3801870	1	6.863	1263350	20.0
n-Hexadecanoic ...	11.933	4.3	ng	406539	4	11.404	1890730	20.0
Phenol, 4,4'-(1...	12.874	8.2	ng	627082	5	14.045	1527840	20.0
Heptafluorobuty...	13.904	14.2	ng	1081910	5	14.045	1527840	20.0
n-Pentadecanol	14.551	2.4	ng	186104	5	14.045	1527840	20.0
Octacosane	15.186	2.1	ng	120497	6	15.533	1164560	20.0
unknown17.680	17.680	2.6	ng	153557	6	15.533	1164560	20.0