

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
 Data File : BF123948.D
 Acq On : 15 May 2021 16:49
 Operator : JU/CG
 Sample : M2392-20
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-07-COMP

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-BF051421.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF123948.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.181	10	16	21	rVB	443277	537124	53.60%	6.611%
2	2.287	29	34	39	rBV	30913	37911	3.78%	0.467%
3	5.116	508	515	521	rBB2	23293	33790	3.37%	0.416%
4	5.510	578	582	585	rBV	931302	847365	84.56%	10.430%
5	6.516	748	753	756	rBV	976442	900174	89.83%	11.080%
6	6.722	785	788	790	rBV	21836	16020	1.60%	0.197%
7	6.898	815	818	822	rBV	335500	289481	28.89%	3.563%
8	7.457	909	913	916	rBV	626988	587772	58.65%	7.235%
9	8.186	1033	1037	1040	rBV	453864	362833	36.21%	4.466%
10	9.263	1215	1220	1223	rBV	1204763	1002115	100.00%	12.335%
11	9.651	1282	1286	1289	rBV	134121	92894	9.27%	1.143%
12	9.939	1332	1335	1339	rVB	490566	402971	40.21%	4.960%
13	10.722	1465	1468	1472	rBV	566397	516559	51.55%	6.358%
14	11.427	1584	1588	1590	rBV	467017	356896	35.61%	4.393%
15	11.451	1590	1592	1595	rVB	27612	20413	2.04%	0.251%
16	11.880	1660	1665	1668	rBV5	15845	25891	2.58%	0.319%
17	11.951	1671	1677	1680	rVB4	61031	58306	5.82%	0.718%
18	12.045	1688	1693	1699	rBV7	6007	13623	1.36%	0.168%
19	12.639	1791	1794	1797	rBV	67233	56393	5.63%	0.694%
20	12.869	1828	1833	1836	rBV	68550	62708	6.26%	0.772%
21	13.016	1853	1858	1861	rVB	1009732	836635	83.49%	10.298%
22	13.910	2006	2010	2013	rBV	157998	152294	15.20%	1.875%
23	14.068	2032	2037	2040	rBV	377567	360068	35.93%	4.432%
24	14.092	2040	2041	2043	rVB	35508	18025	1.80%	0.222%
25	14.545	2115	2118	2121	rBV5	17191	16724	1.67%	0.206%
26	14.868	2167	2173	2176	rBV7	14442	27920	2.79%	0.344%
27	15.121	2211	2216	2222	rVB	37175	74861	7.47%	0.921%
28	15.427	2265	2268	2271	rVB3	22379	26220	2.62%	0.323%
29	15.492	2275	2279	2285	rBV2	23103	31249	3.12%	0.385%
30	15.557	2285	2290	2295	rBV2	203952	270455	26.99%	3.329%
31	16.057	2371	2375	2378	rBV6	11915	16930	1.69%	0.208%
32	16.104	2378	2383	2387	rVV7	15535	27945	2.79%	0.344%
33	16.621	2467	2471	2474	rBV5	8272	11781	1.18%	0.145%
34	16.745	2489	2492	2495	rBV5	7022	11793	1.18%	0.145%
35	17.504	2616	2621	2626	rVB7	9898	19996	2.00%	0.246%

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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-BF051421.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

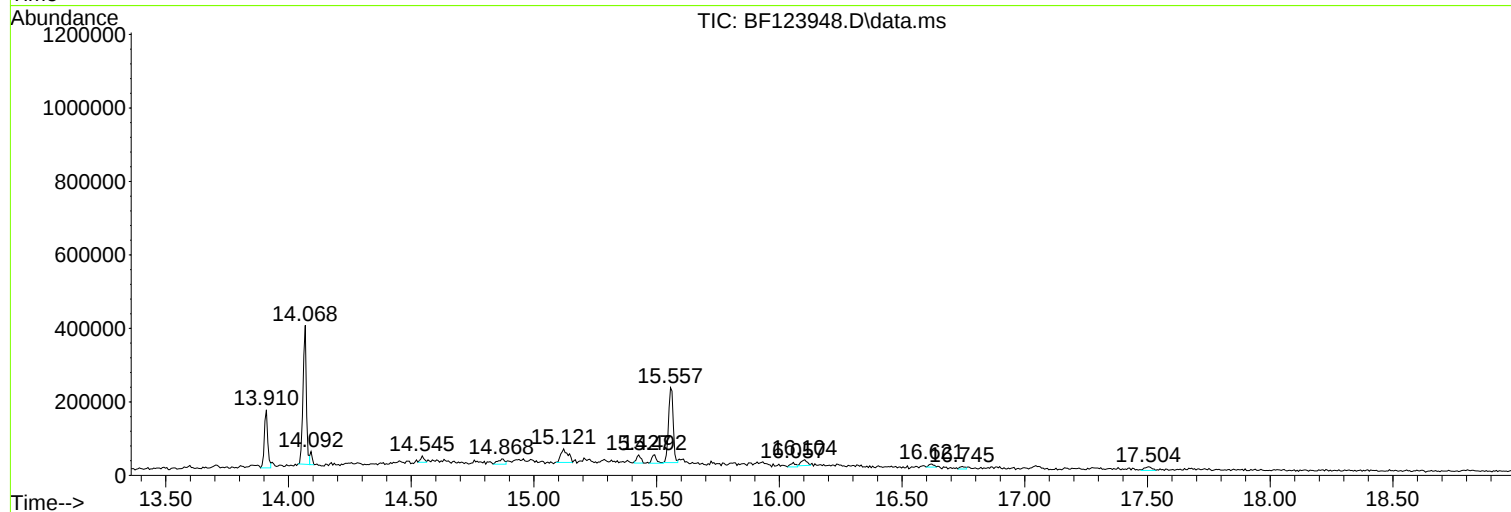
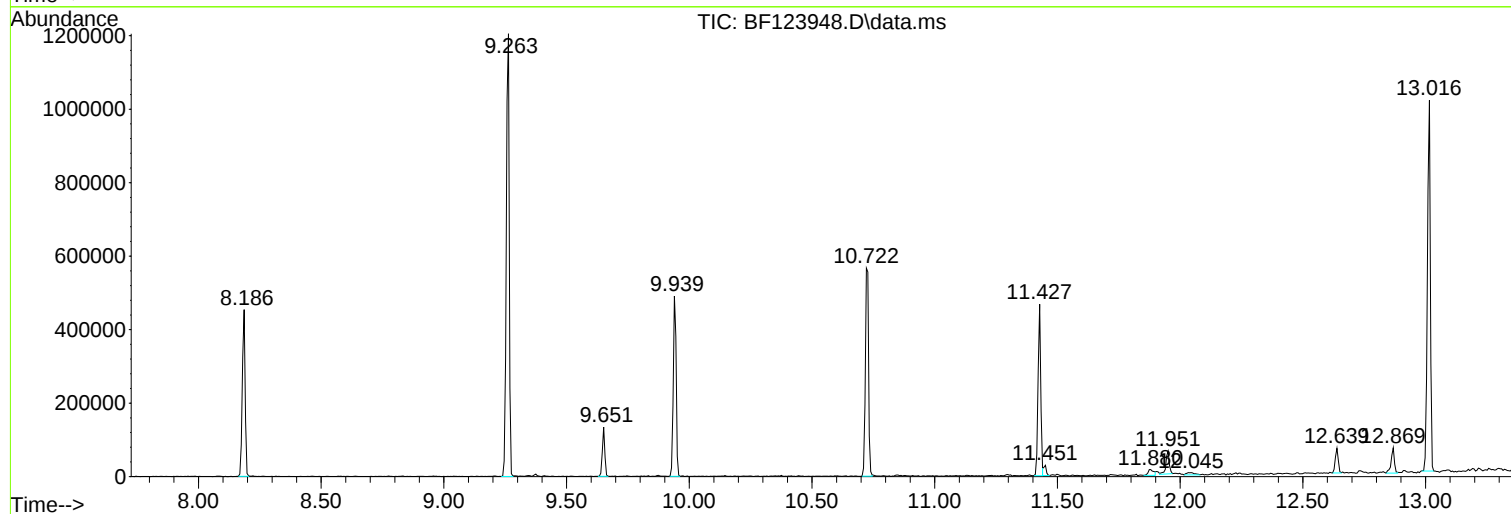
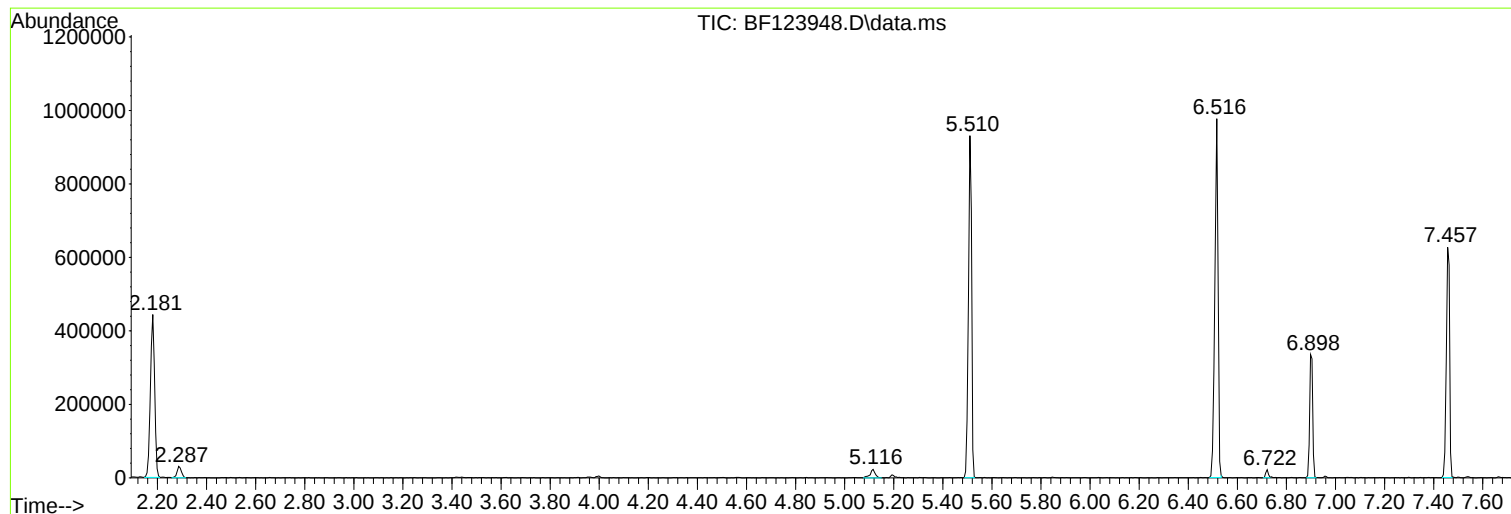
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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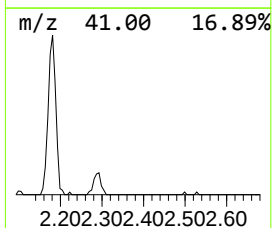
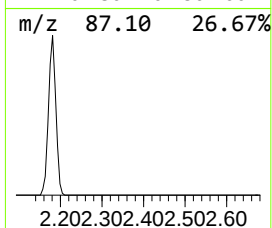
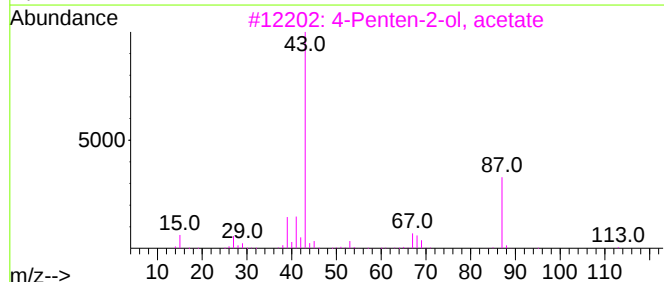
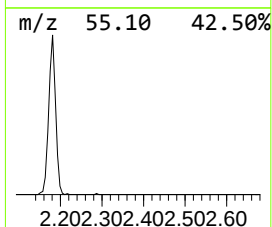
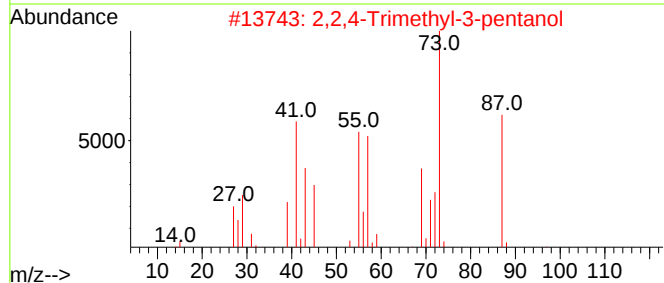
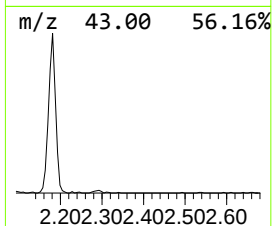
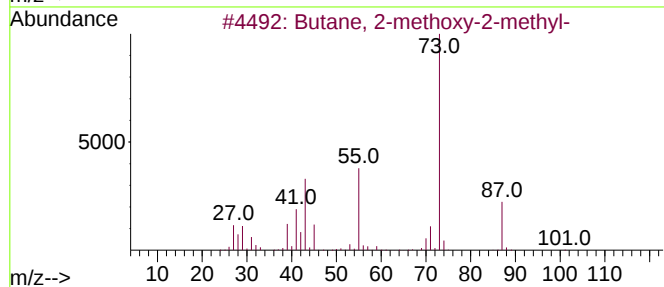
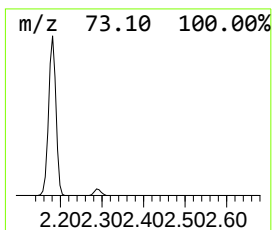
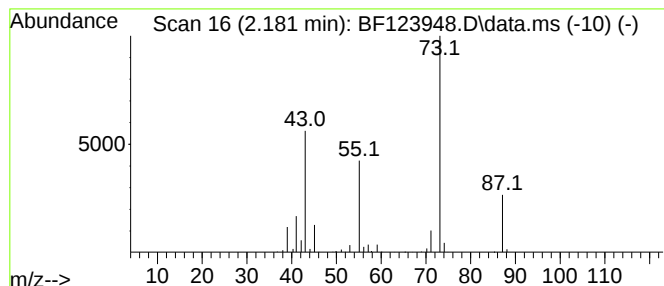
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
2.181	37.11 ng	537124	1,4-Dichlorobenzene-d4	6.904

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			4-Penten-2-ol, acetate	128	C7H12O2	1000352-31-5	10
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	9



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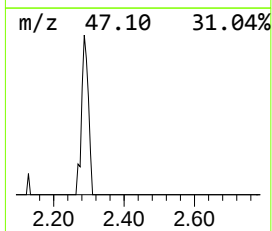
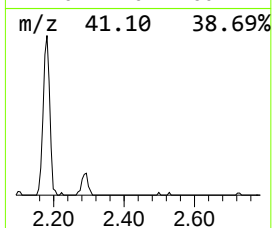
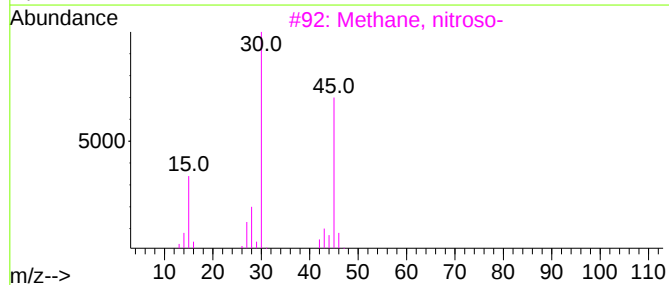
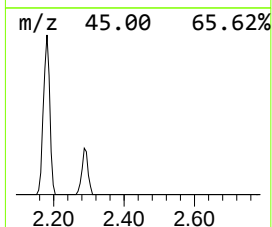
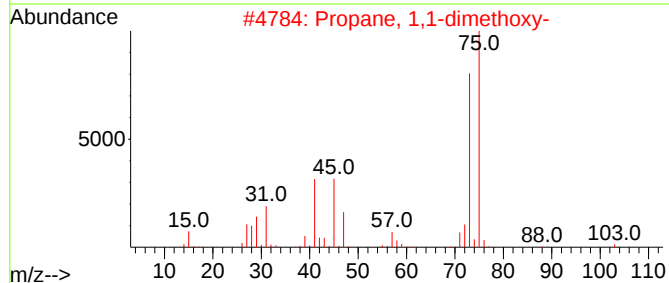
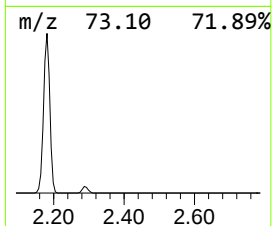
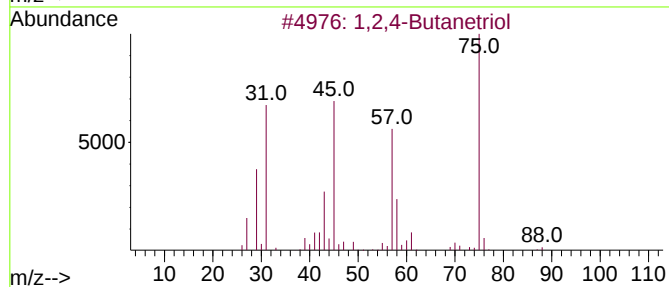
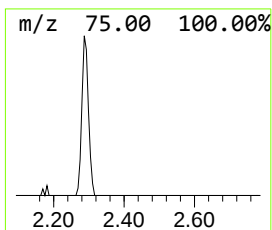
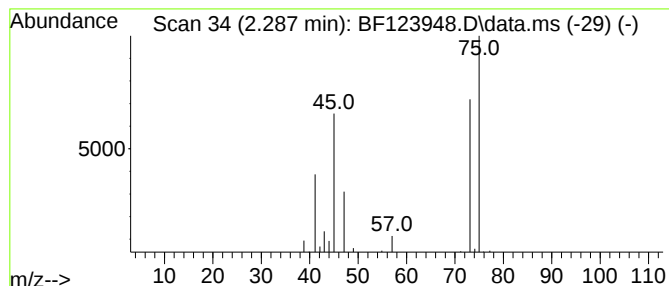
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown2.287 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.287	2.62 ng	37911	1,4-Dichlorobenzene-d4	6.904

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,2,4-Butanetriol	106	C4H10O3	003068-00-6	9
2		Propane, 1,1-dimethoxy-	104	C5H12O2	004744-10-9	9
3		Methane, nitroso-	45	CH3NO	000865-40-7	7
4		Ethanethioamide	75	C2H5NS	000062-55-5	5
5		Formamide, N-methylthio	75	C2H5NS	018952-41-5	5



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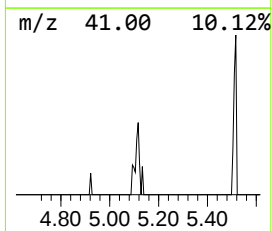
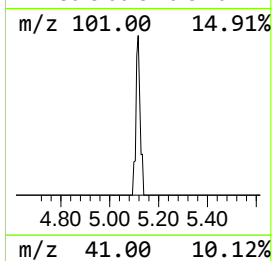
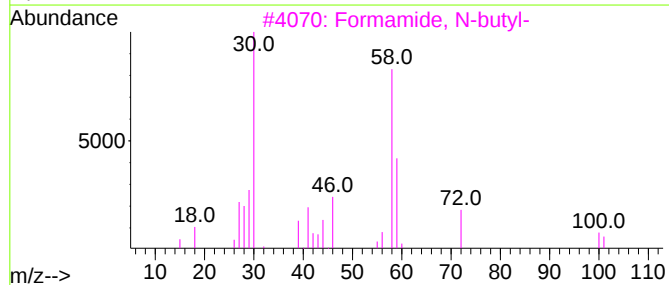
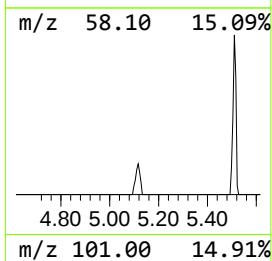
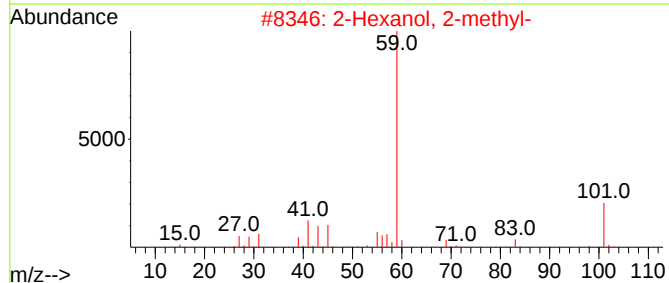
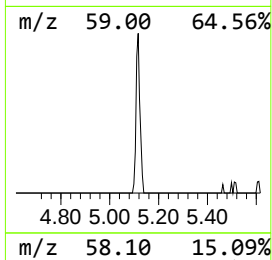
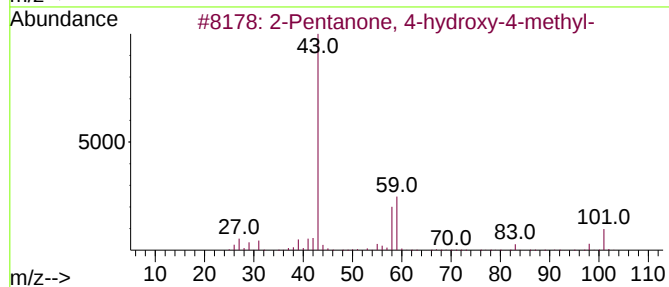
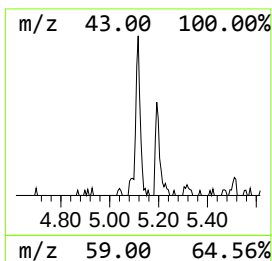
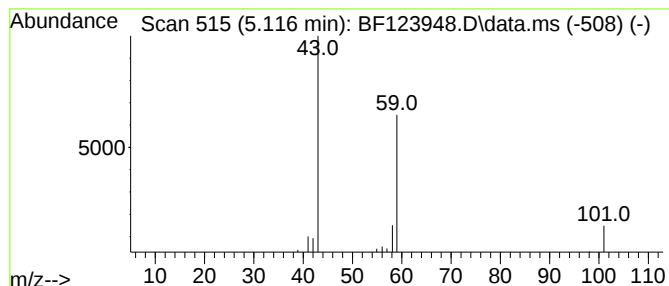
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.116	2.33 ng	33790	1,4-Dichlorobenzene-d4	6.904

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	33
2		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	25
3		Formamide, N-butyl-	101	C5H11NO	000871-71-6	9
4		2-Nonanone, 9-hydroxy-	158	C9H18O2	025368-56-3	9
5		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	9



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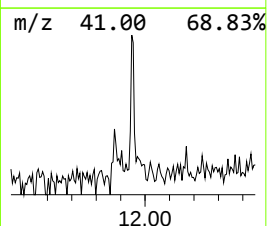
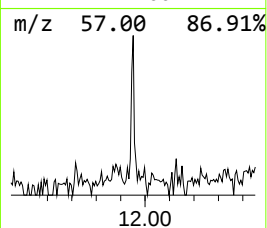
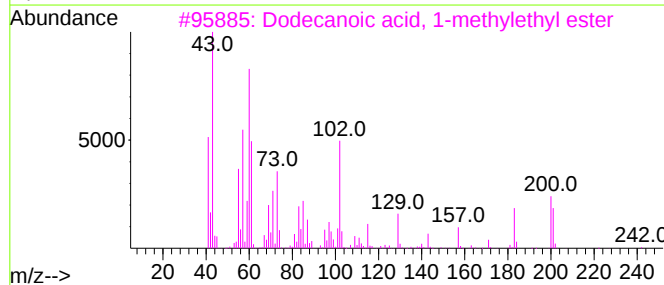
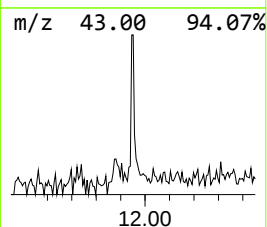
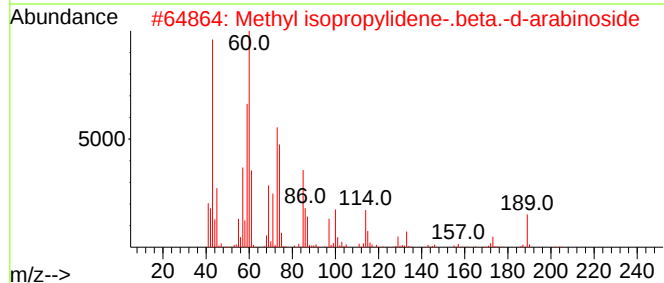
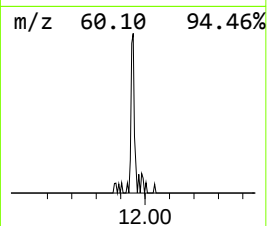
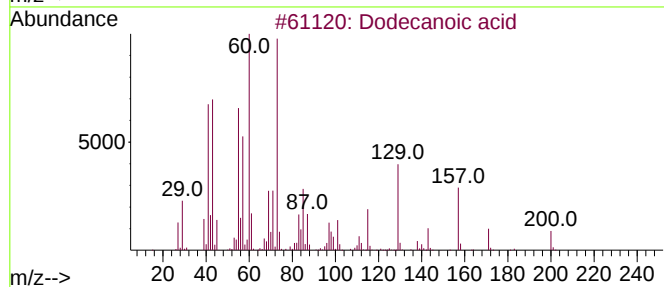
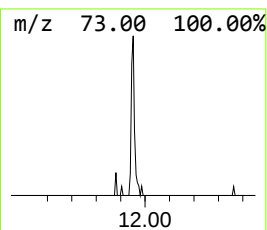
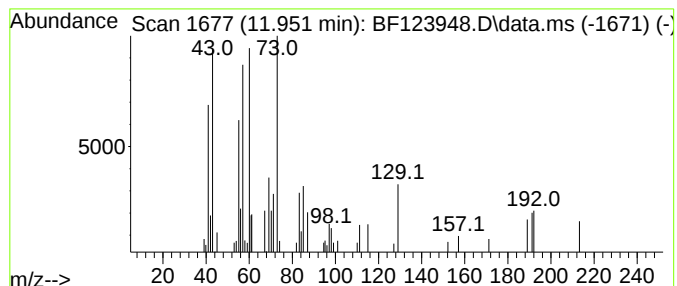
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Dodecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.951	3.27 ng	58306	Phenanthrene-d10	11.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dodecanoic acid	200	C12H24O2	000143-07-7	50
2			Methyl isopropylidene-.beta.-d-a...	204	C9H16O5	1000129-88-1	50
3			Dodecanoic acid, 1-methylethyl e...	242	C15H30O2	010233-13-3	47
4			Undecanoic acid	186	C11H22O2	000112-37-8	47
5			Trehalose	342	C12H22O11	000099-20-7	43



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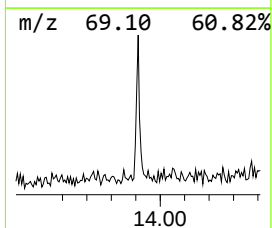
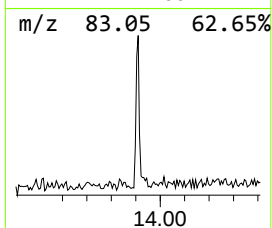
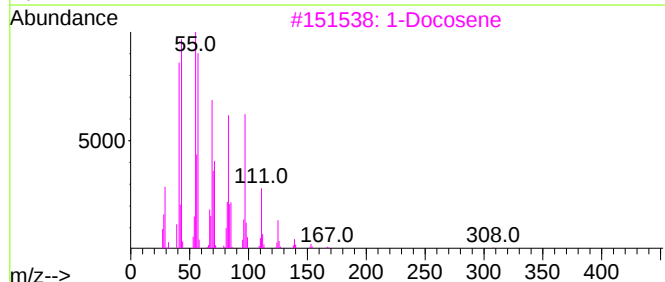
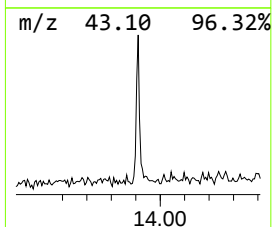
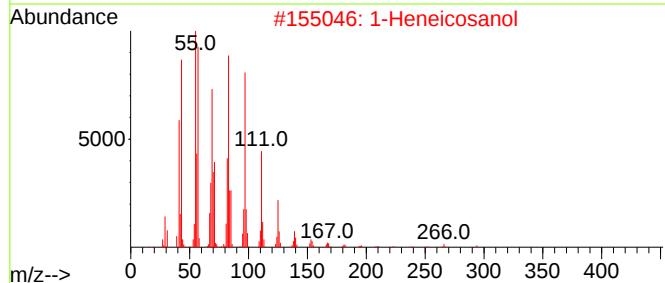
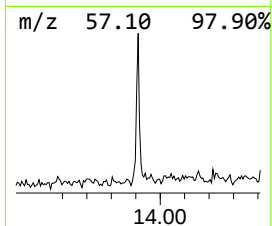
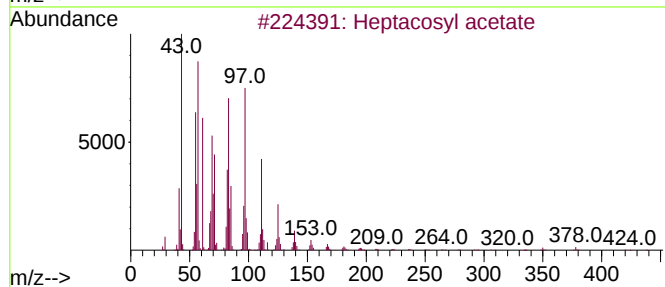
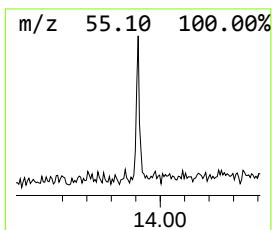
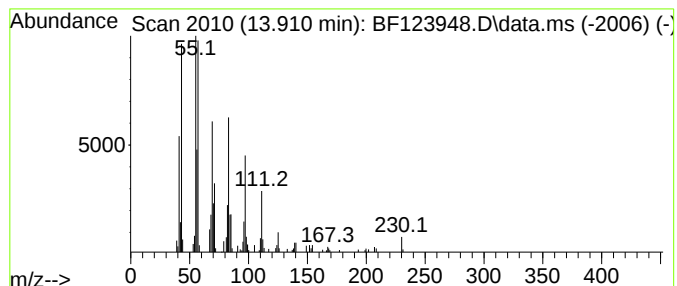
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Heptacosyl acetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.910	8.46 ng	152294	Chrysene-d12	14.069

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptacosyl acetate	438	C29H58O2	1000351-78-2	80
2			1-Heneicosanol	312	C21H44O	015594-90-8	72
3			1-Docosene	308	C22H44	001599-67-3	68
4			Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	68
5			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	68



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123948.D
Acq On : 15 May 2021 16:49
Operator : JU/CG
Sample : M2392-20
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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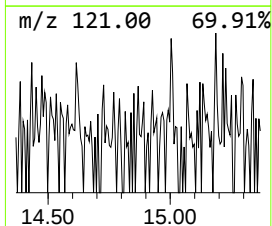
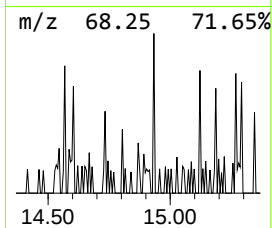
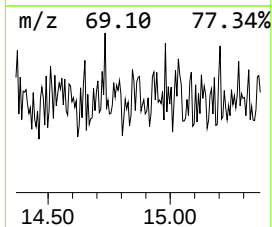
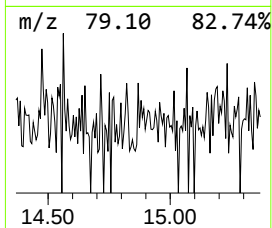
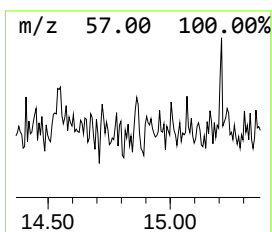
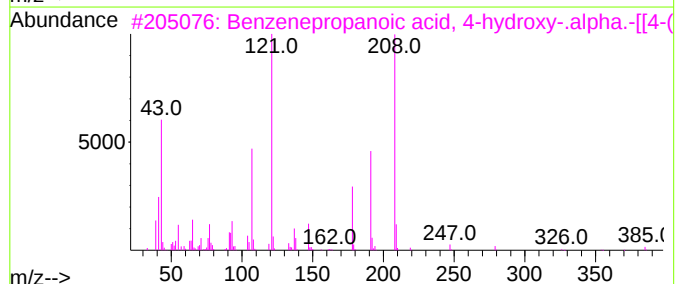
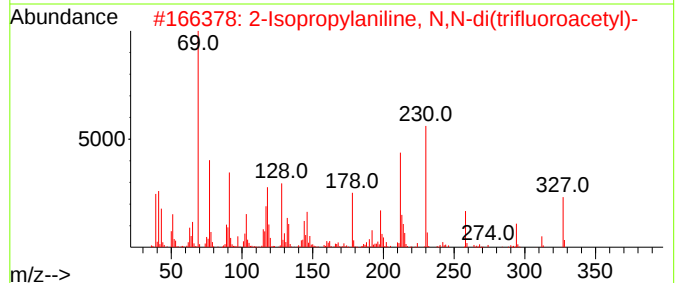
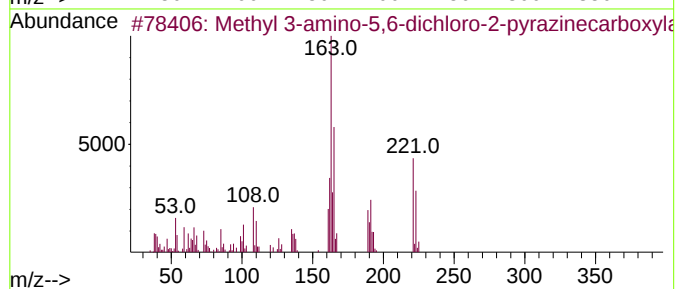
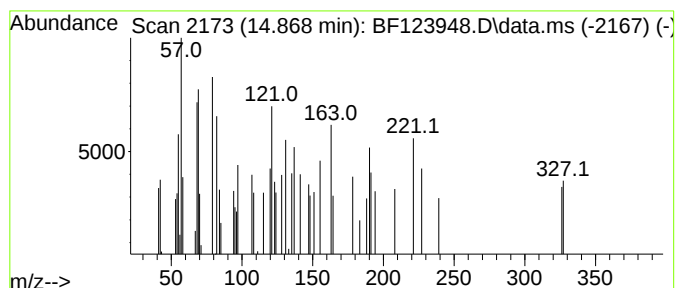
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown14.868 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.868	2.06 ng	27920	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methyl 3-amino-5,6-dichloro-2-py...	221	C6H5Cl2N3O2	001458-18-0	14
2			2-Isopropylaniline, N,N-di(trifl...	327	C13H11F6NO2	1000328-31-8	9
3			Benzenepropanoic acid, 4-hydroxy...	385	C22H27NO5	1000320-15-8	9
4			1-Chloro-4-(2-chloro-2-fluoroeth...	190	C8H5Cl2F	1000305-36-3	9
5			O-Ethyl seleno-3-methylbutyrate	194	C7H14OSe	1000074-76-5	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
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Sample : M2392-20
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-COMP

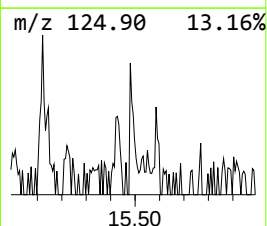
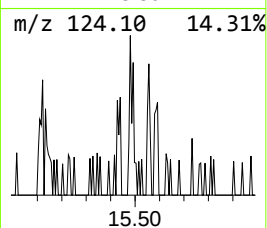
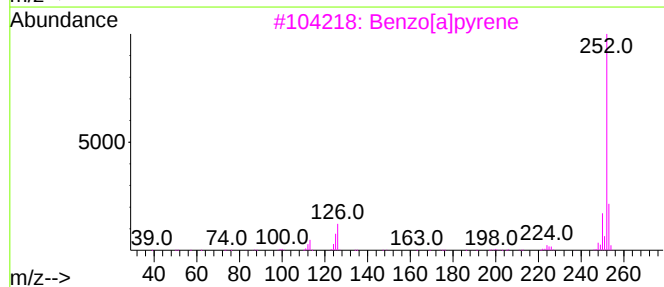
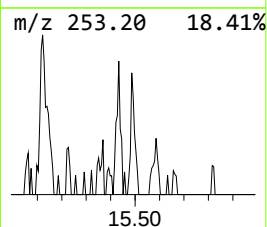
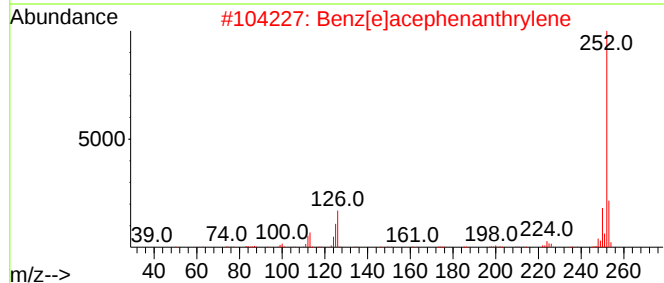
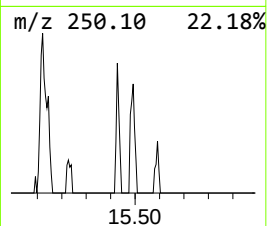
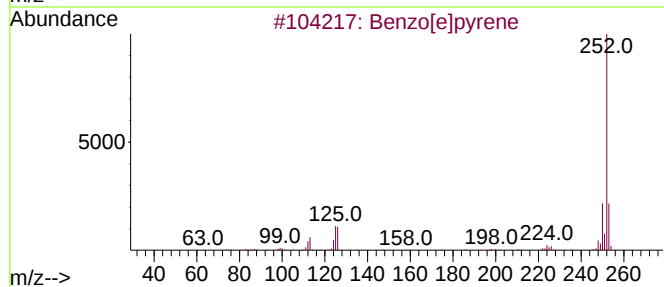
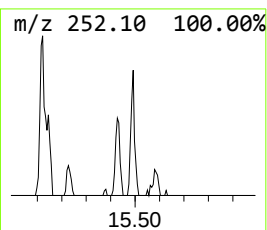
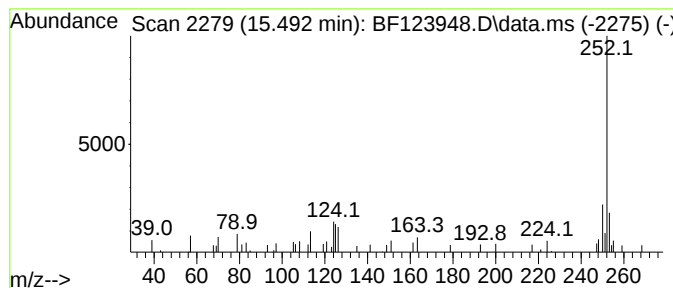
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzo[e]pyrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.492	2.31 ng	31249	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzo[e]pyrene	252	C20H12	000192-97-2	81
2			Benz[e]acephenanthrylene	252	C20H12	000205-99-2	81
3			Benzo[a]pyrene	252	C20H12	000050-32-8	72
4			Perylene	252	C20H12	000198-55-0	64
5			Benzo[k]fluoranthene	252	C20H12	000207-08-9	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
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Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-COMP

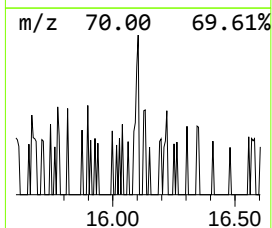
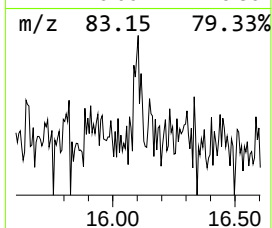
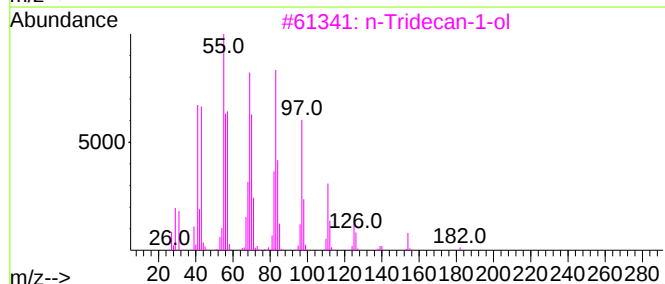
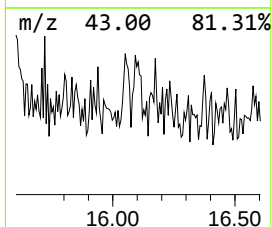
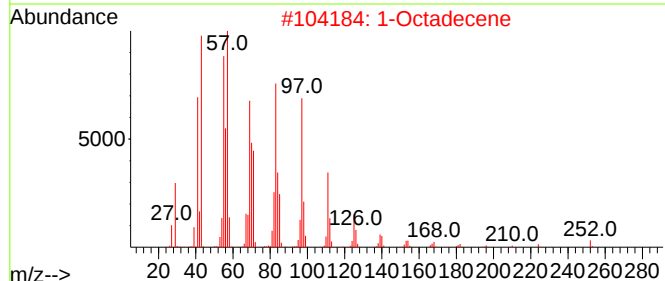
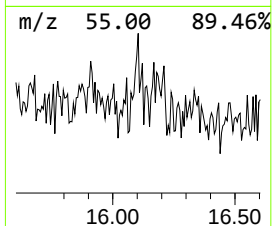
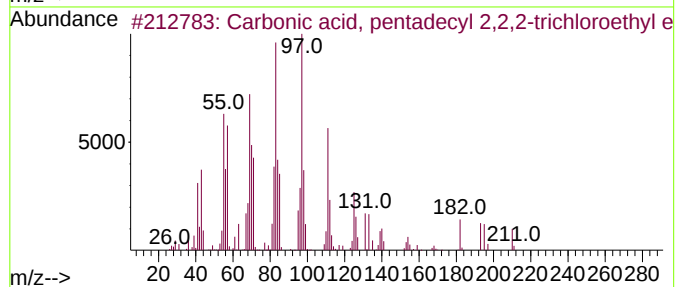
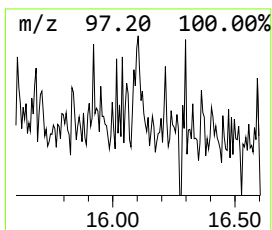
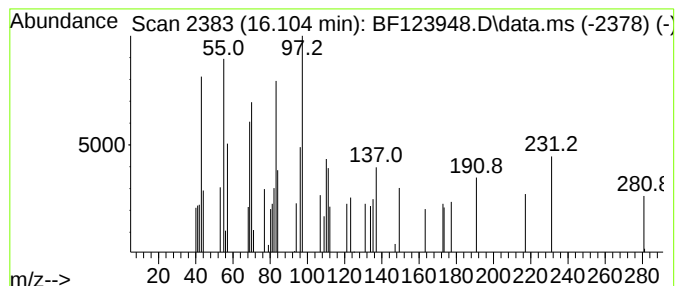
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown16.104 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.104	2.07 ng	27945	Perylene-d12	15.563

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonic acid, pentadecyl 2,2,2-...	402	C18H33Cl3O3	1000314-56-1	43
2			1-Octadecene	252	C18H36	000112-88-9	43
3			n-Tridecan-1-ol	200	C13H28O	000112-70-9	35
4			Cyclododecane	168	C12H24	000294-62-2	35
5			4-Trifluoromethylbenzoic acid, t...	372	C21H31F3O2	1000280-05-3	27



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF051521\
Data File : BF123948.D
Acq On : 15 May 2021 16:49
Operator : JU/CG
Sample : M2392-20
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-07-COMP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_F\METHODS\8270-BF051421.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...	2.181	37.1	ng	537124	1	6.904	289481	20.0
unknown2.287	2.287	2.6	ng	37911	1	6.904	289481	20.0
2-Pentanone, 4-...	5.116	2.3	ng	33790	1	6.904	289481	20.0
Dodecanoic acid	11.951	3.3	ng	58306	4	11.427	356896	20.0
Heptacosyl acetate	13.910	8.5	ng	152294	5	14.069	360068	20.0
unknown14.868	14.868	2.1	ng	27920	6	15.563	270455	20.0
Benzo[e]pyrene	15.492	2.3	ng	31249	6	15.563	270455	20.0
unknown16.104	16.104	2.1	ng	27945	6	15.563	270455	20.0