

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110123\
 Data File : BF136085.D
 Acq On : 01 Nov 2023 19:33
 Operator : CG\JU
 Sample : 05142-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PSC-124037

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-BF103023.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF136085.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.122	3	6	11	rVB	622064	726014	16.52%	2.176%
2	4.446	394	401	405	rBV	1857634	2209616	50.29%	6.623%
3	5.069	499	507	519	rVB	1579571	2487191	56.61%	7.455%
4	5.463	568	574	577	rBV	3727317	4061459	92.44%	12.173%
5	5.845	635	639	645	rVB	158455	127806	2.91%	0.383%
6	6.463	737	744	747	rBV	3389666	3948806	89.88%	11.836%
7	6.651	773	776	786	rVB	62396	63705	1.45%	0.191%
8	6.822	802	805	808	rBV	1160469	861697	19.61%	2.583%
9	7.387	896	901	904	rBV	2597303	2625219	59.75%	7.869%
10	8.104	1019	1023	1026	rBV	1392784	1131555	25.75%	3.392%
11	9.186	1202	1207	1210	rBV	5148953	4393655	100.00%	13.169%
12	9.298	1223	1226	1230	rVB	69484	56911	1.30%	0.171%
13	9.863	1318	1322	1325	rBV	1397858	1192371	27.14%	3.574%
14	10.651	1452	1456	1460	rBV	2448057	2393073	54.47%	7.173%
15	11.351	1571	1575	1578	rBV	1231625	1055511	24.02%	3.164%
16	11.892	1663	1667	1677	rBV2	424104	433357	9.86%	1.299%
17	12.569	1779	1782	1786	rBV	95305	96373	2.19%	0.289%
18	12.680	1798	1801	1811	rBV2	127175	157520	3.59%	0.472%
19	12.798	1820	1821	1825	rVB	75283	58623	1.33%	0.176%
20	12.957	1843	1848	1851	rBV	3509272	3174424	72.25%	9.515%
21	13.904	2005	2009	2019	rVB5	53517	135950	3.09%	0.407%
22	14.010	2022	2027	2030	rBV	1046040	924906	21.05%	2.772%
23	14.498	2107	2110	2113	rBV2	53183	55384	1.26%	0.166%
24	14.657	2134	2137	2141	rBV	103731	97847	2.23%	0.293%
25	14.815	2161	2164	2168	rVB2	47850	59700	1.36%	0.179%
26	15.168	2221	2224	2229	rVB	49892	54458	1.24%	0.163%
27	15.504	2275	2281	2289	rBV	599395	780442	17.76%	2.339%

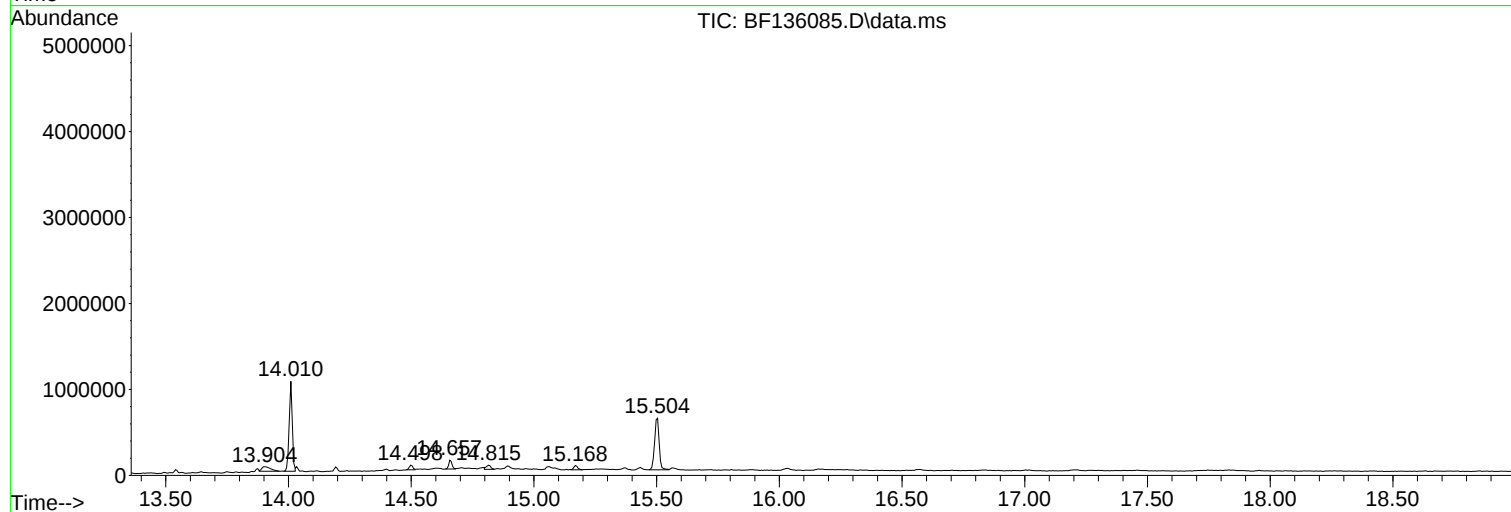
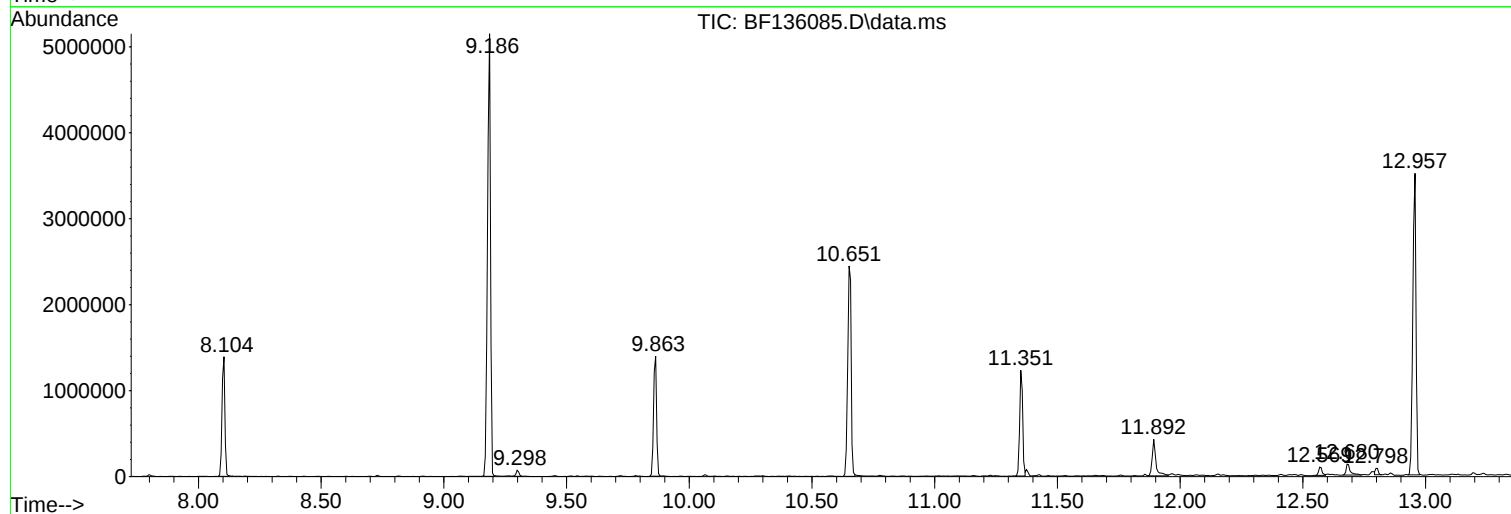
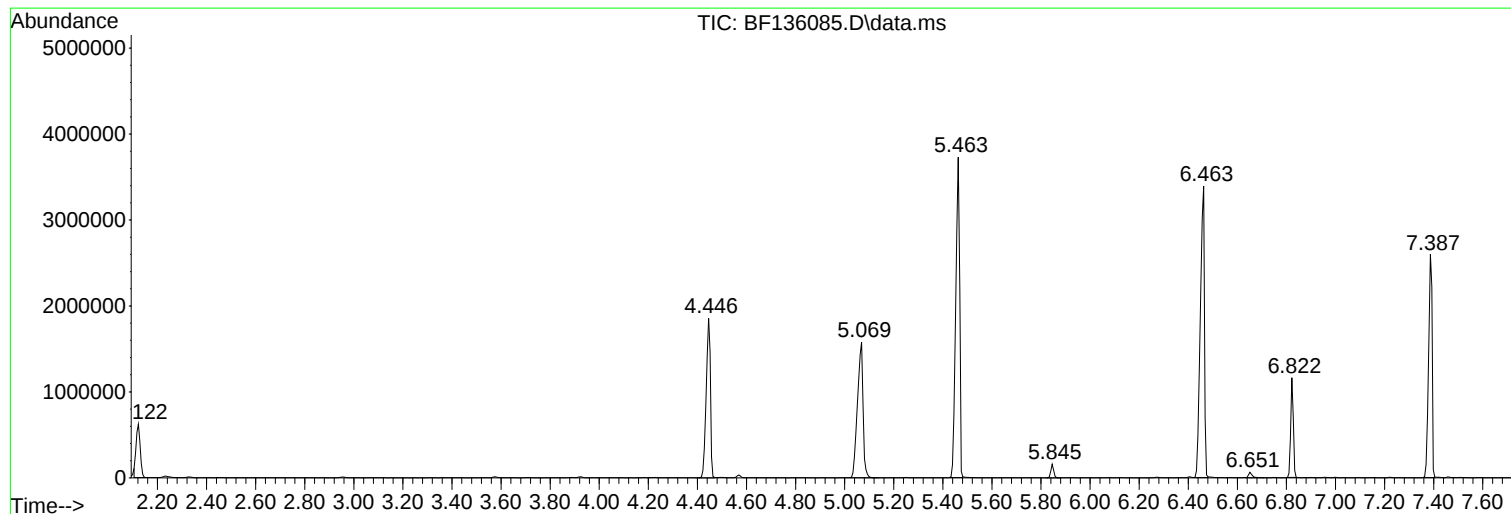
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ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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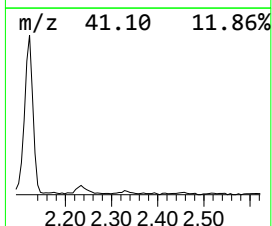
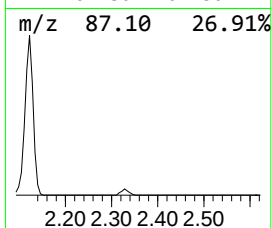
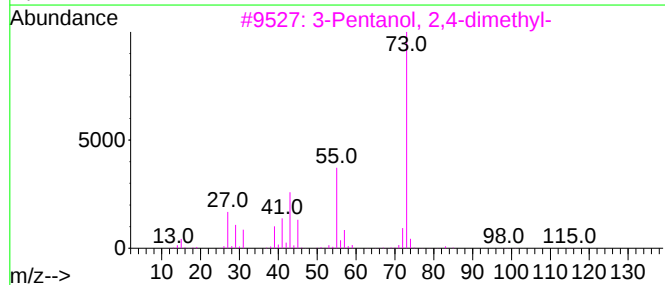
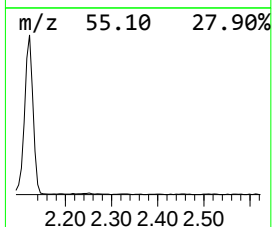
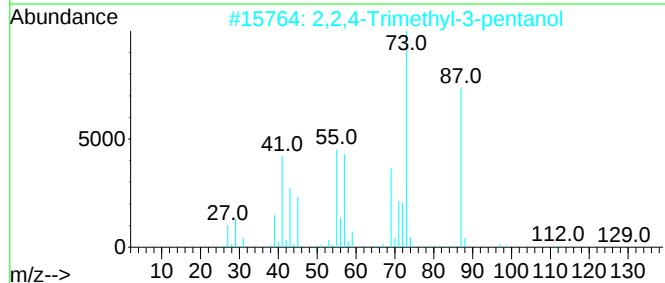
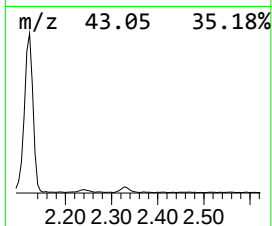
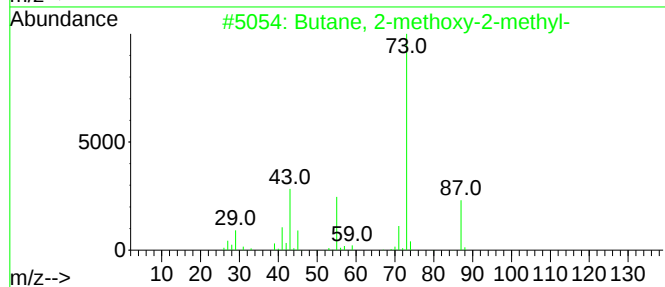
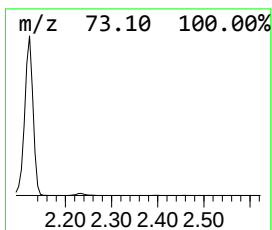
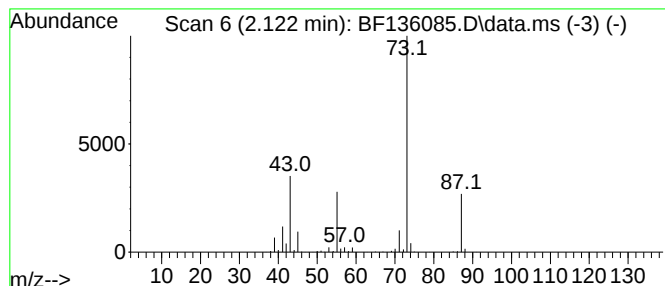
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	16.85 ng	726014	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
4			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	22
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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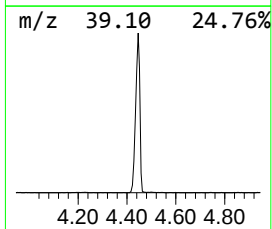
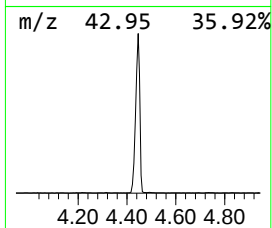
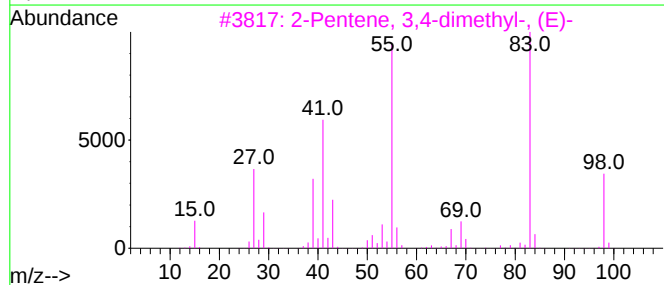
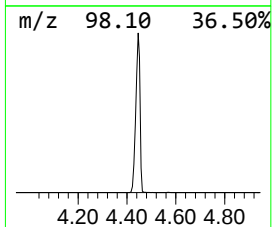
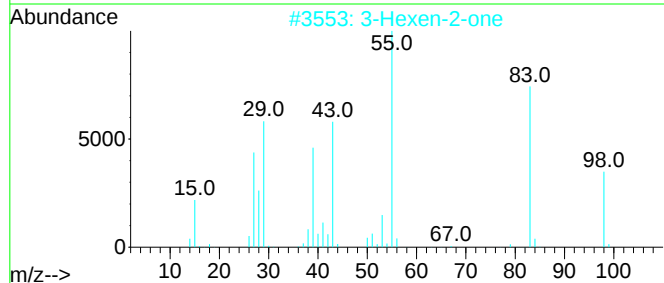
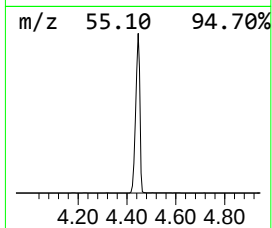
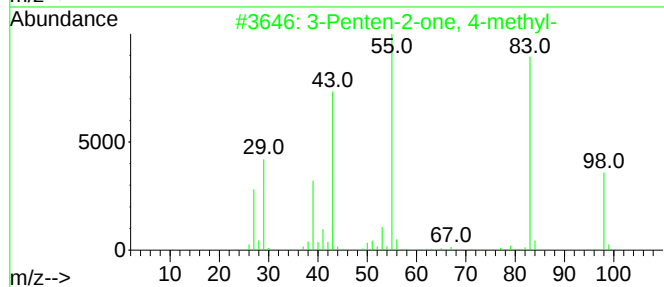
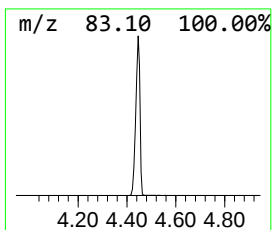
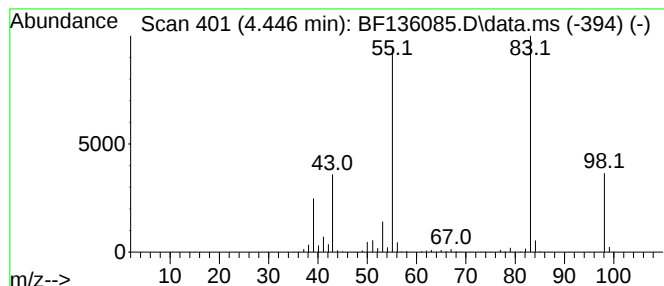
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.446	51.29 ng	2209620	1,4-Dichlorobenzene-d4	6.822

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		3-Hexen-2-one	98	C6H10O	000763-93-9	91
3		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	90
4		2-Pentene, 3,4-dimethyl-, (Z)-	98	C7H14	004914-91-4	86
5		2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	80



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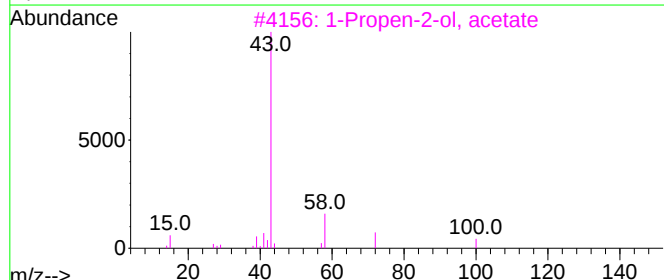
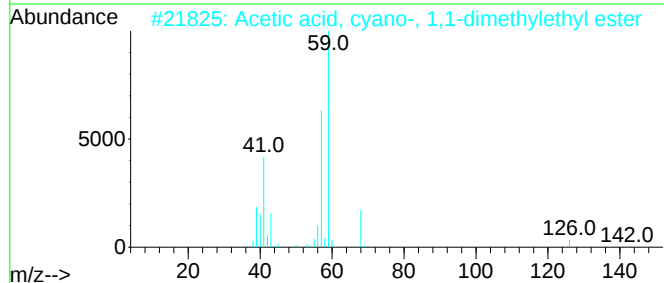
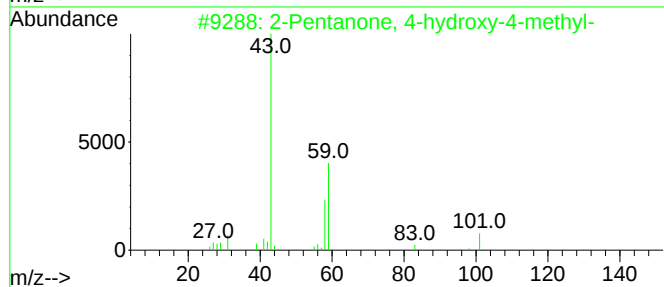
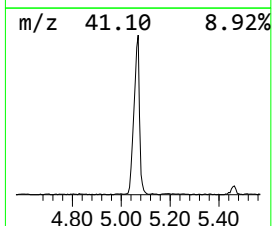
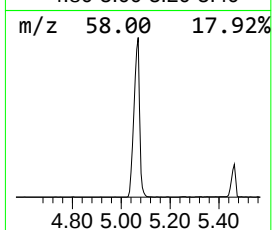
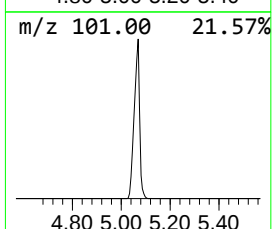
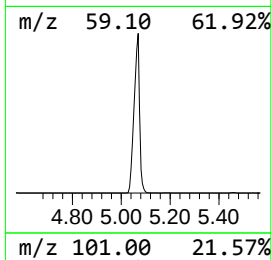
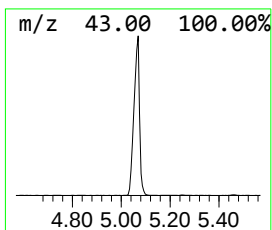
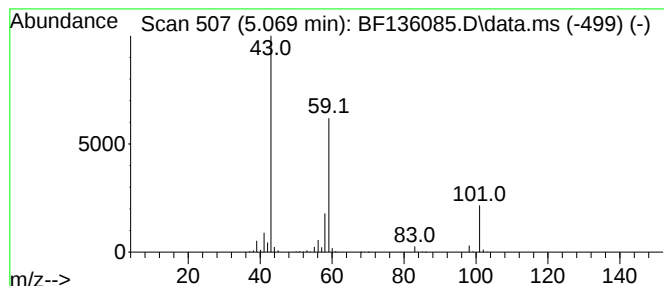
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.069	57.73 ng	2487190	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
3			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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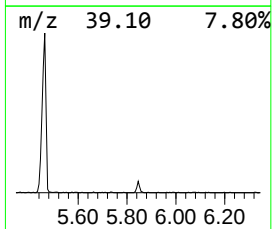
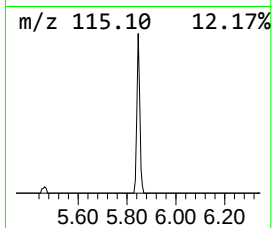
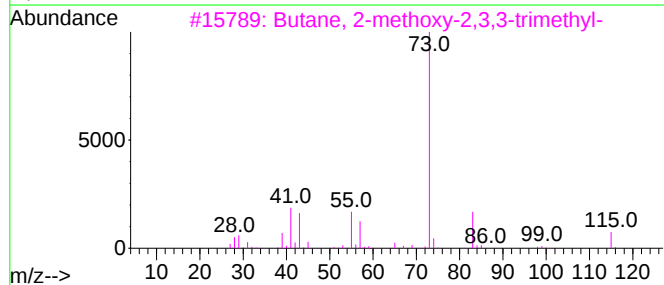
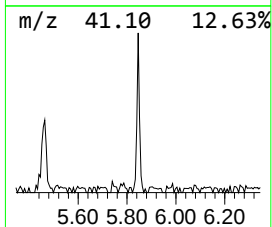
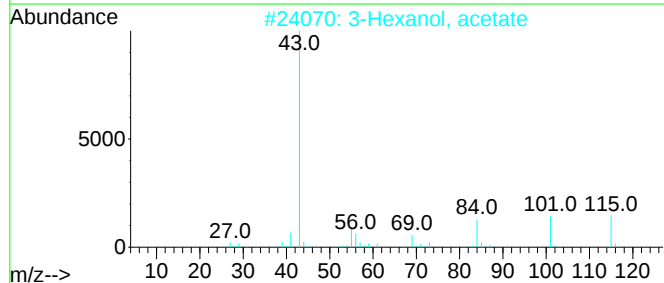
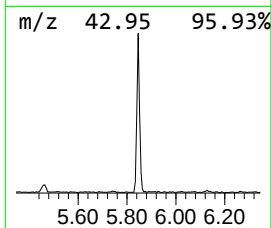
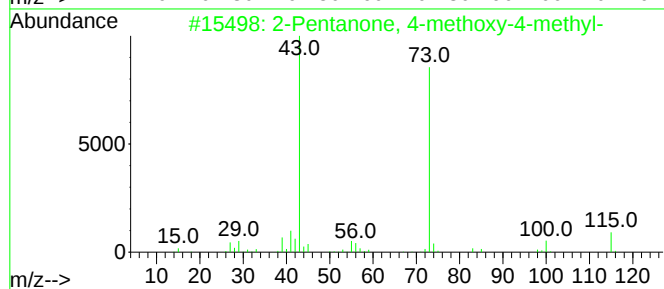
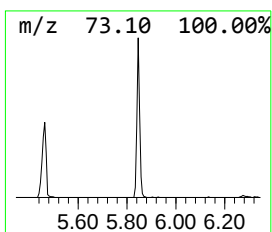
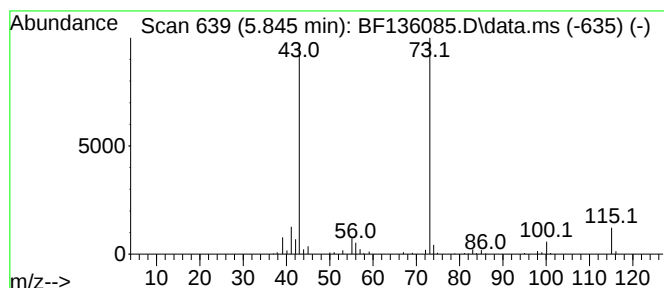
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Peak Number 4 2-Pentanone, 4-methoxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.845	2.97 ng	127806	1,4-Dichlorobenzene-d4	6.822

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-methoxy-4-methyl-	130	C7H14O2	000107-70-0	83
2			3-Hexanol, acetate	144	C8H16O2	040780-64-1	37
3			Butane, 2-methoxy-2,3,3-trimethyl-	130	C8H18O	027705-21-1	23
4			1,3-Dioxolane, 2-pentadecyl-	284	C18H36O2	004360-57-0	12
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	12



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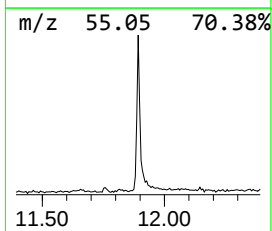
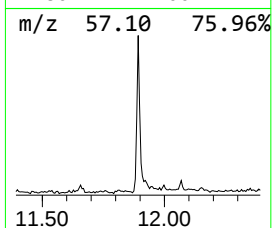
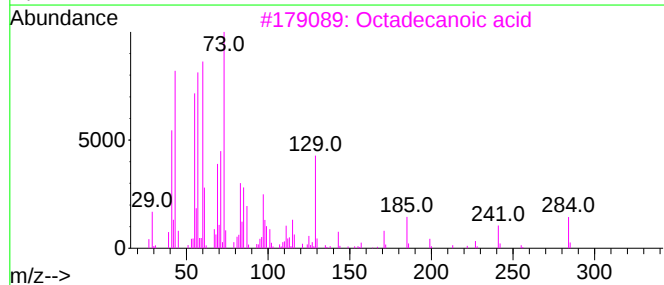
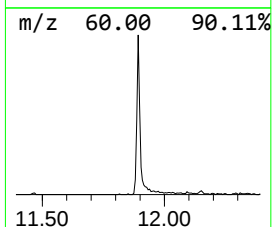
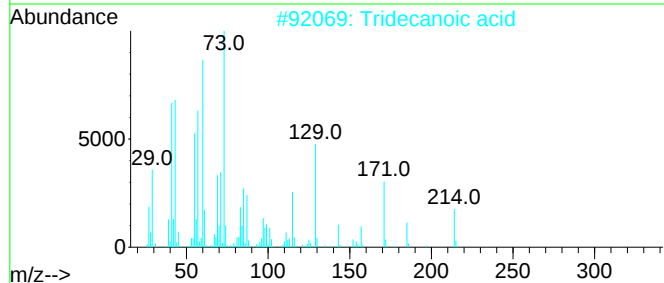
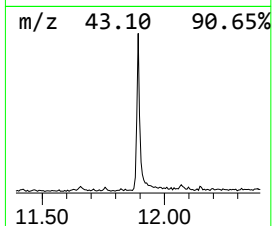
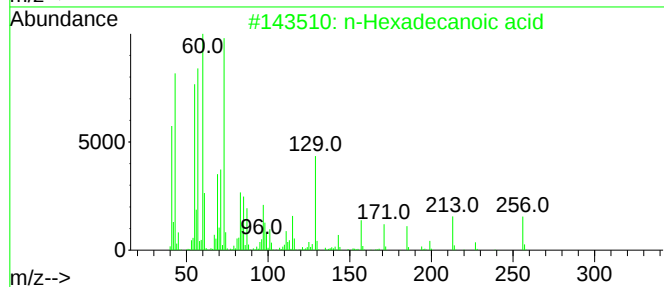
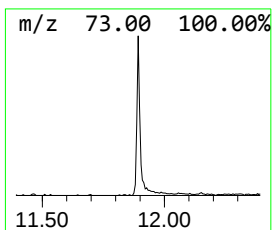
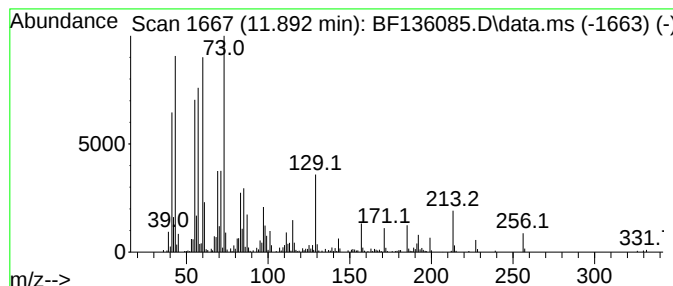
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.892	8.21 ng	433357	Phenanthrene-d10	11.351

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	95
3			Octadecanoic acid	284	C18H36O2	000057-11-4	93
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	91
5			Pentadecanoic acid	242	C15H30O2	001002-84-2	87



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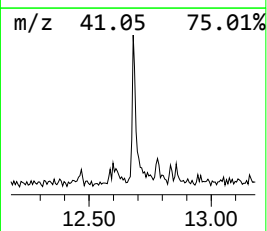
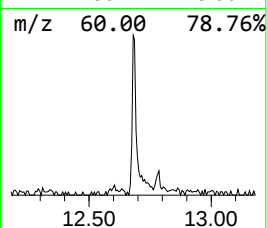
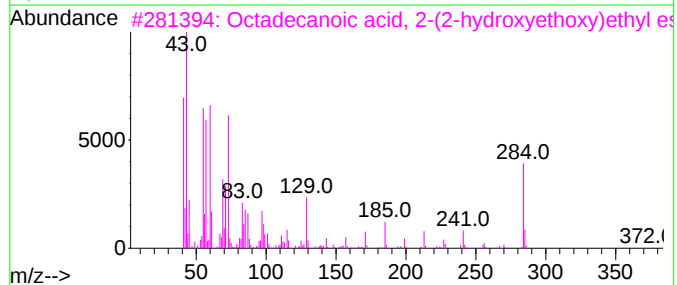
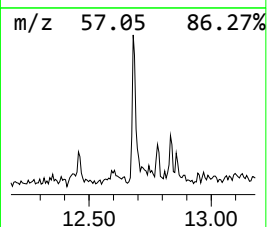
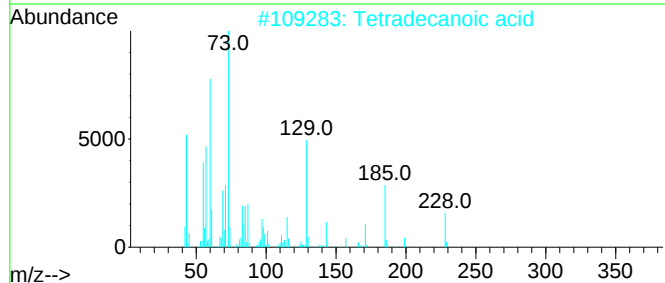
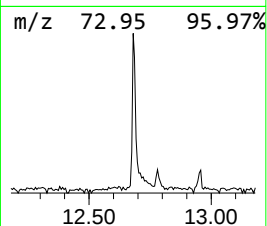
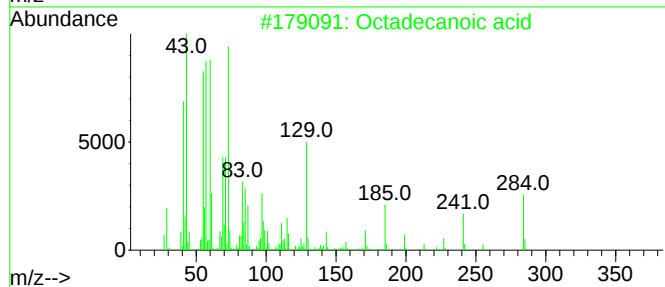
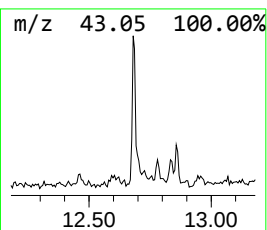
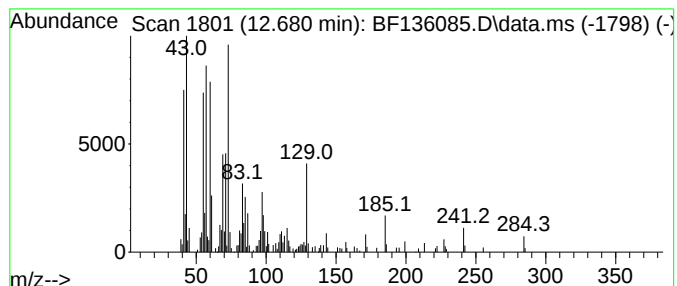
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.680	2.98 ng	157520	Phenanthrene-d10	11.351

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	90
5			n-Decanoic acid	172	C10H20O2	000334-48-5	76



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110123\
Data File : BF136085.D
Acq On : 01 Nov 2023 19:33
Operator : CG\JU
Sample : 05142-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC-124037

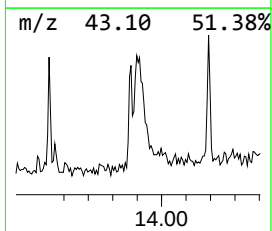
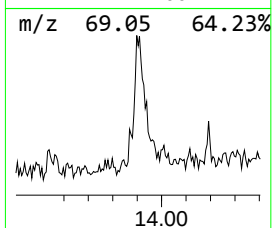
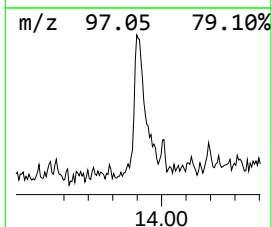
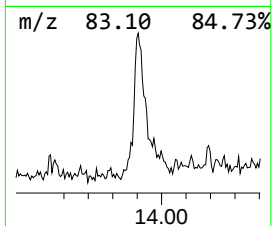
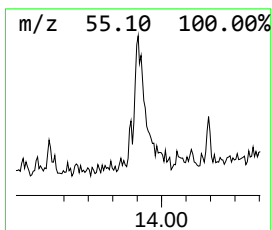
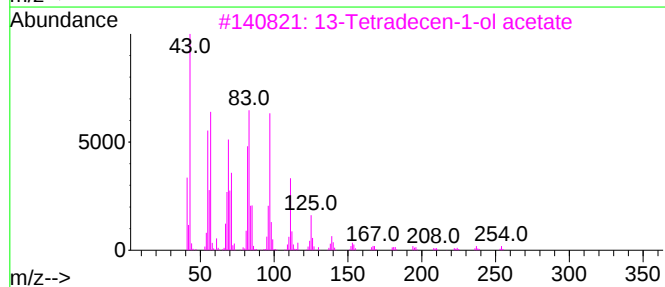
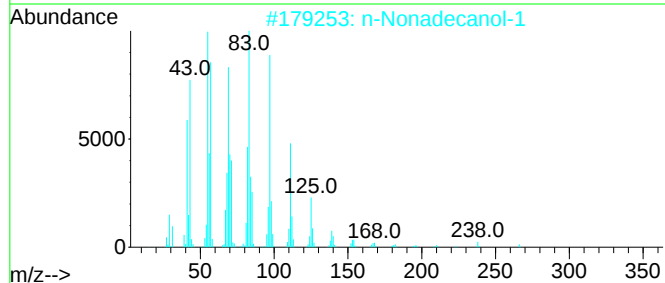
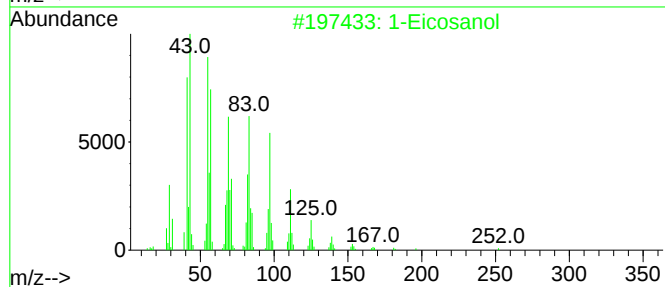
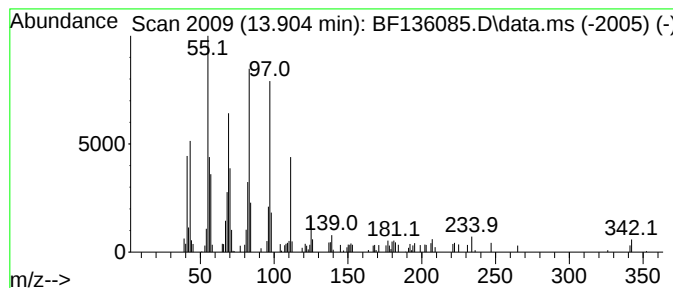
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 1-Eicosanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.904	2.94 ng	135950	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Eicosanol	298	C20H42O	000629-96-9	90
2			n-Nonadecanol-1	284	C19H40O	001454-84-8	87
3			13-Tetradecen-1-ol acetate	254	C16H30O2	056221-91-1	86
4			1-Docosene	308	C22H44	001599-67-3	83
5			1-Heneicosanol	312	C21H44O	015594-90-8	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110123\
Data File : BF136085.D
Acq On : 01 Nov 2023 19:33
Operator : CG\JU
Sample : 05142-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC-124037

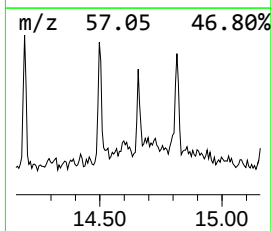
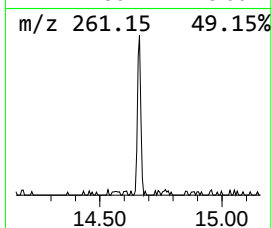
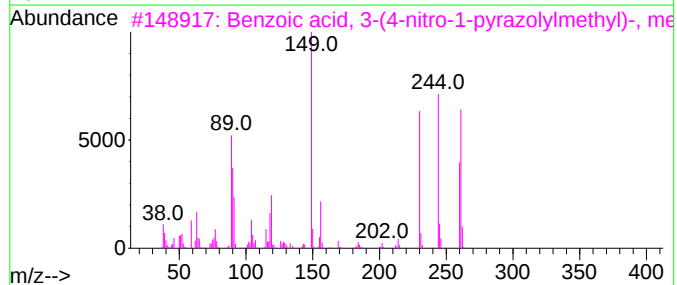
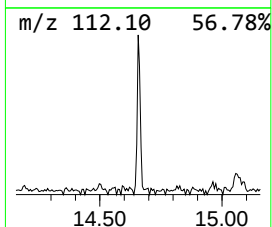
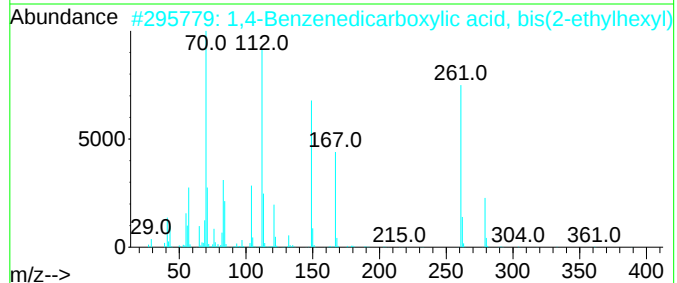
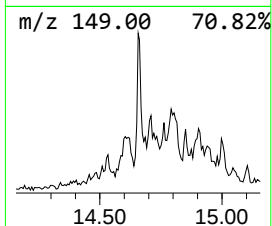
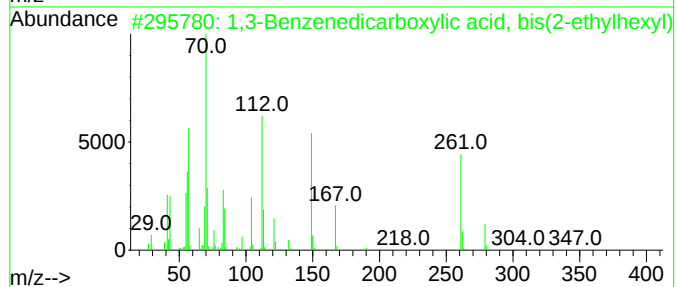
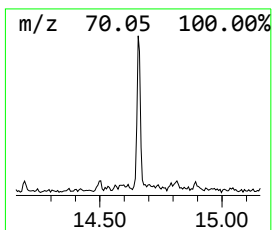
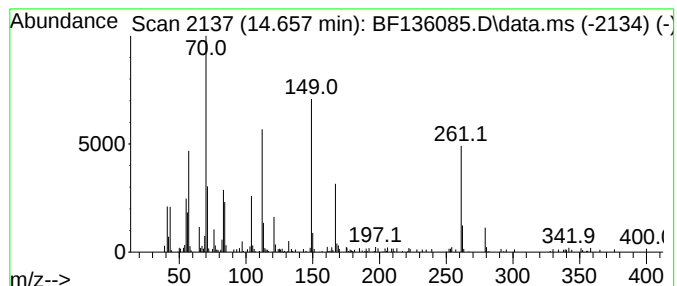
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 1,3-Benzenedicarboxylic aci... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.657	2.12 ng	97847	Chrysene-d12	14.010

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,3-Benzenedicarboxylic acid, bi...	390	C24H3804	000137-89-3	90
2			1,4-Benzenedicarboxylic acid, bi...	390	C24H3804	006422-86-2	58
3			Benzoic acid, 3-(4-nitro-1-pyraz...	261	C12H11N3O4	1000273-84-4	22
4			Bis(2-ethylhexyl) phthalate	390	C24H3804	000117-81-7	22
5			Phthalic acid, 6-ethyloct-3-yl 2...	418	C26H42O4	1000315-53-8	14



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF110123\
Data File : BF136085.D
Acq On : 01 Nov 2023 19:33
Operator : CG\JU
Sample : 05142-01
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
PSC-124037

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF103023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.122	16.9	ng	726014	1	6.822	861697	20.0
3-Penten-2-one,...	4.446	51.3	ng	2209620	1	6.822	861697	20.0
2-Pentanone, 4-...	5.069	57.7	ng	2487190	1	6.822	861697	20.0
2-Pentanone, 4-...	5.845	3.0	ng	127806	1	6.822	861697	20.0
n-Hexadecanoic ...	11.892	8.2	ng	433357	4	11.351	1055510	20.0
Octadecanoic acid	12.680	3.0	ng	157520	4	11.351	1055510	20.0
1-Eicosanol	13.904	2.9	ng	135950	5	14.010	924906	20.0
1,3-Benzenedica...	14.657	2.1	ng	97847	5	14.010	924906	20.0