

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110420\
 Data File : BP003805.D
 Acq On : 04 Nov 2020 14:28
 Operator : CG/JU
 Sample : L3971-06
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_P
 ClientSampleId :
 PT-ACIDS-WP

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_P\METHODS\8270-BP110320.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BP003805.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.099	29	36	47	rBV	405580	772012	7.81%	0.792%
2	3.193	47	52	58	rVV	329436	368694	3.73%	0.378%
3	5.287	403	408	417	rVB	72329	105900	1.07%	0.109%
4	5.811	490	497	515	rBV	3187381	4782493	48.41%	4.907%
5	7.463	768	778	780	rBV	2911114	5323104	53.88%	5.462%
6	7.493	780	783	795	rVB	3695869	5112242	51.74%	5.245%
7	7.863	838	846	854	rBV	2441884	3838270	38.85%	3.938%
8	8.293	912	919	929	rBV	470736	754098	7.63%	0.774%
9	8.752	990	997	1005	rBV	1668927	2580675	26.12%	2.648%
10	9.075	1044	1052	1065	rBV	2388616	3736805	37.82%	3.834%
11	9.457	1108	1117	1125	rBV	1967299	3303780	33.44%	3.390%
12	10.228	1240	1248	1253	rBV	1833058	2970958	30.07%	3.048%
13	10.293	1253	1259	1273	rVB	3587080	5651062	57.20%	5.798%
14	10.781	1333	1342	1357	rBV	3810737	6313322	63.90%	6.478%
15	11.128	1390	1401	1408	rBV	602857	996277	10.08%	1.022%
16	11.304	1424	1431	1440	rBV	1306615	2125949	21.52%	2.181%
17	12.381	1606	1614	1628	rBV	1511454	2251014	22.78%	2.310%
18	13.363	1773	1781	1788	rBV	4610567	6900020	69.84%	7.080%
19	13.434	1788	1793	1804	rVV	1211994	1765090	17.87%	1.811%
20	13.540	1804	1811	1821	rVB	4837798	6878058	69.62%	7.057%
21	14.910	2037	2044	2051	rBV2	836357	1241273	12.56%	1.274%
22	14.992	2051	2058	2083	rBV	1979583	2806554	28.41%	2.880%
23	16.016	2224	2232	2247	rBV	3095783	4237331	42.89%	4.348%
24	16.392	2288	2296	2313	rBV	3421807	4851768	49.11%	4.978%
25	17.304	2443	2451	2470	rBV	1702158	2359034	23.88%	2.420%
26	17.639	2501	2508	2517	rBV	1039843	1432027	14.49%	1.469%
27	20.127	2925	2931	2940	rBV	8399955	9879797	100.00%	10.137%
28	21.657	3185	3191	3202	rBV	1188355	1593397	16.13%	1.635%
29	23.280	3462	3467	3473	rVB	97138	146358	1.48%	0.150%
30	23.910	3568	3574	3582	rBV	129175	229948	2.33%	0.236%
31	24.121	3603	3610	3621	rVB	770384	1506718	15.25%	1.546%
32	24.621	3690	3695	3704	rVB	117897	234315	2.37%	0.240%
33	25.457	3830	3837	3845	rBV	99383	238883	2.42%	0.245%
34	26.427	3996	4002	4015	rVB4	62839	177425	1.80%	0.182%

Sum of corrected areas: 97464651

Instrument :

BNA_P

ClientSampleId :

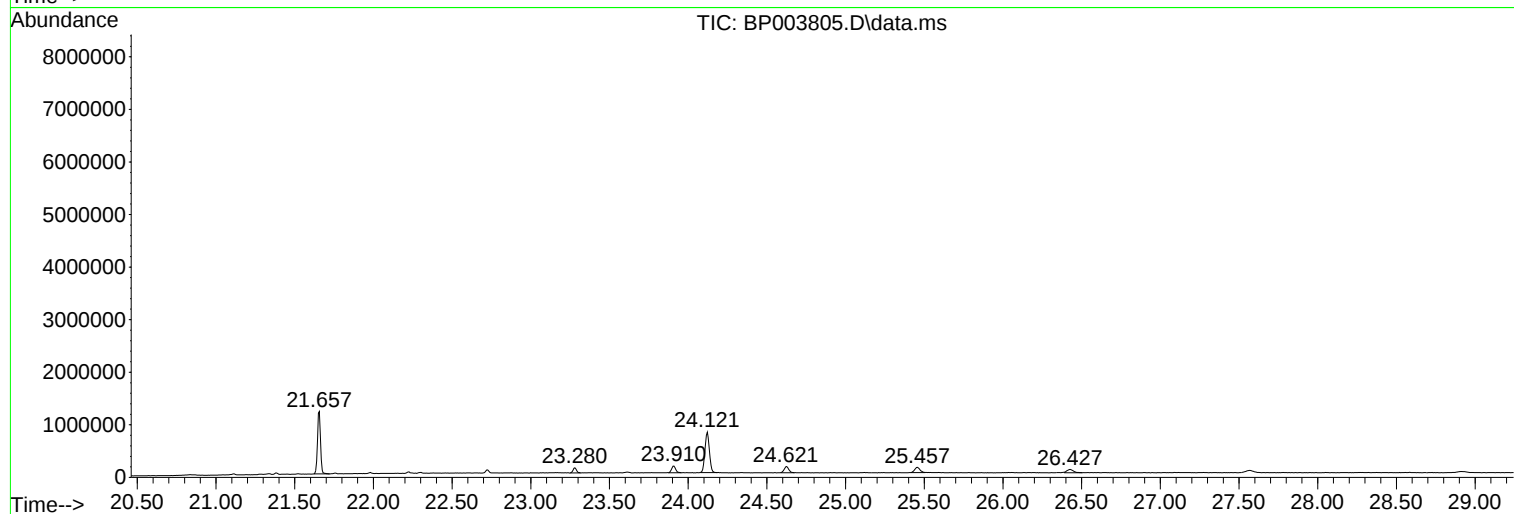
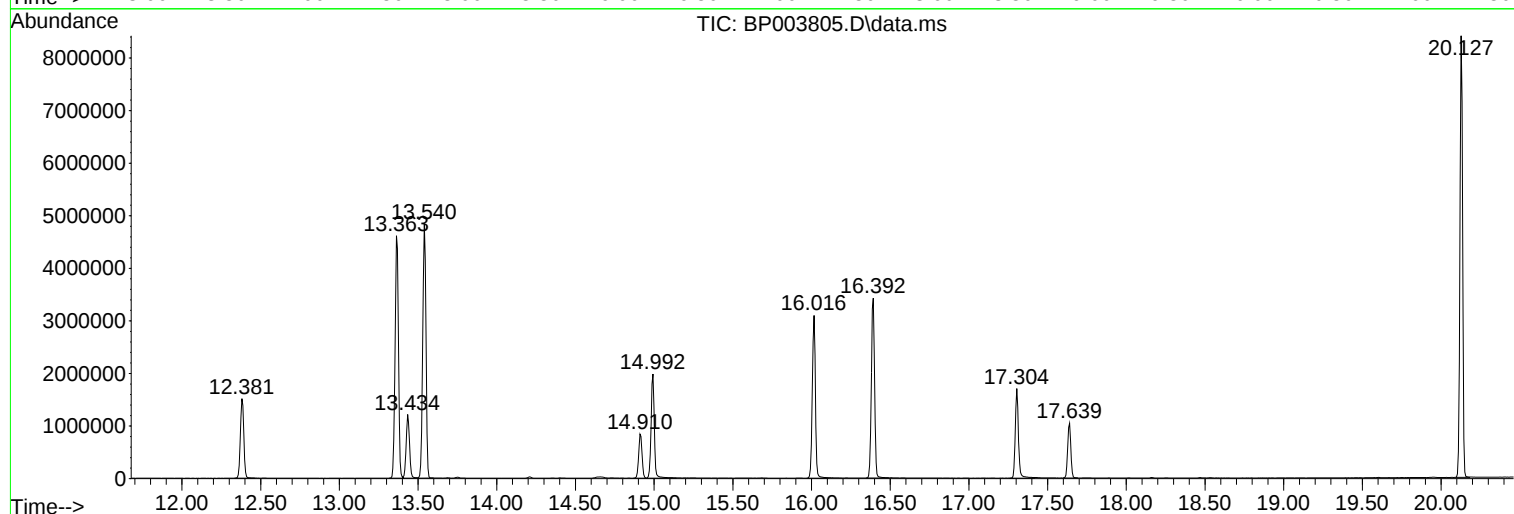
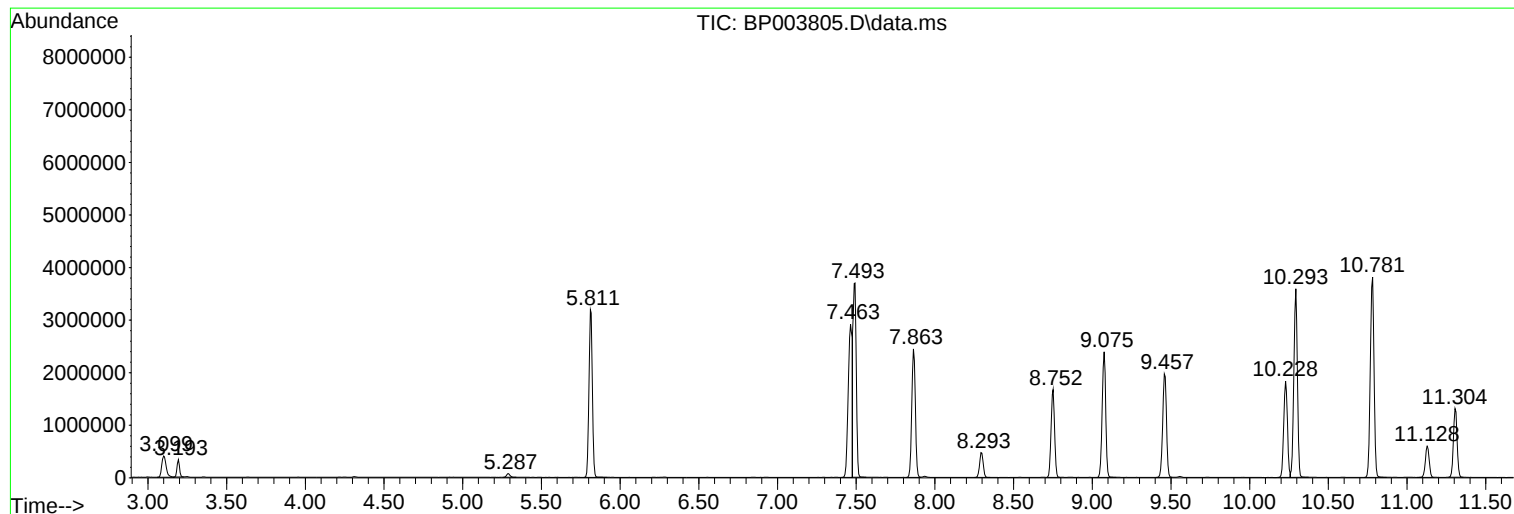
PT-ACIDS-WP

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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.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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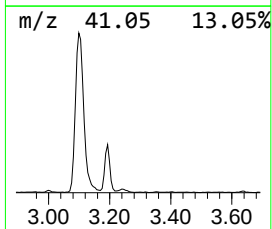
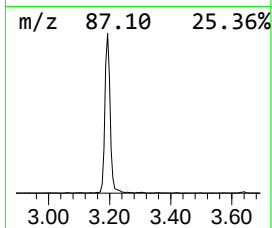
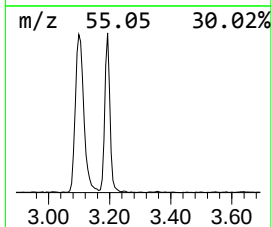
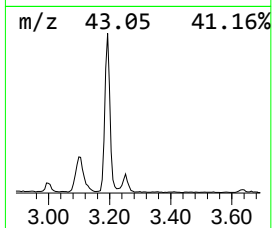
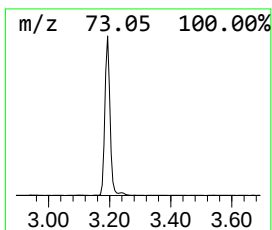
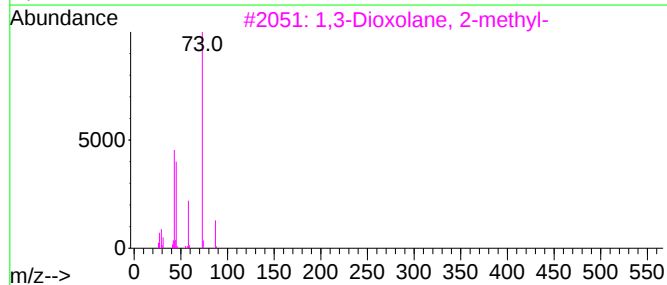
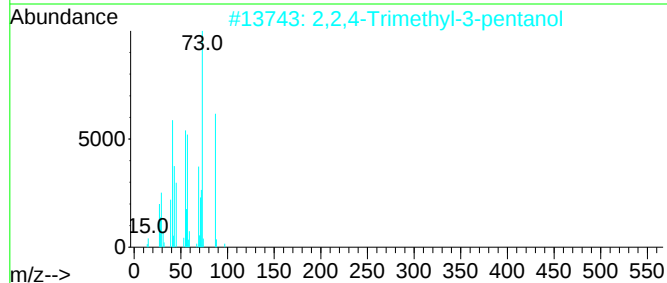
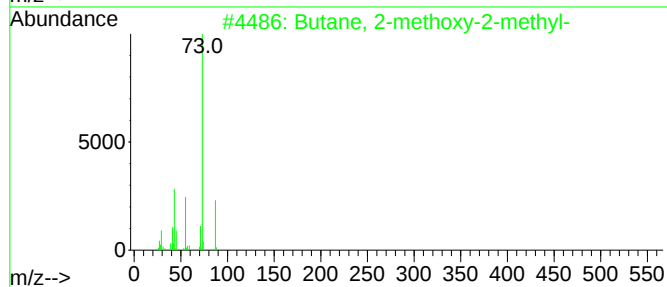
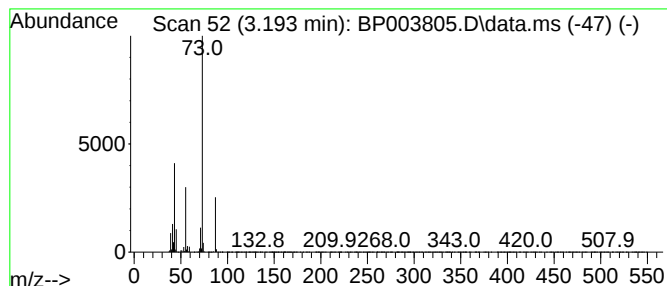
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.193	9.78 ng	368694	1,4-Dichlorobenzene-d4	8.293

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	39
3		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	16
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	12



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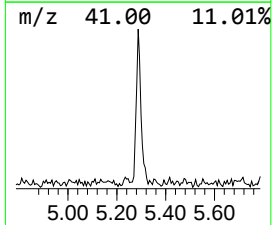
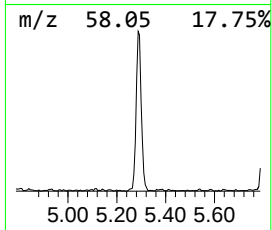
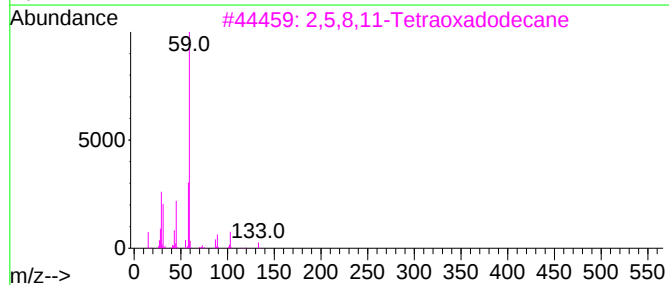
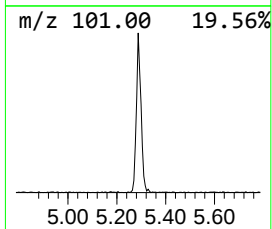
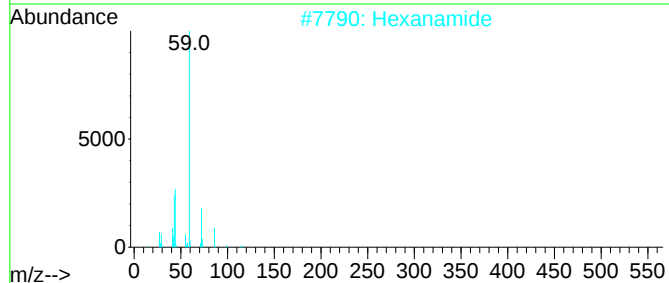
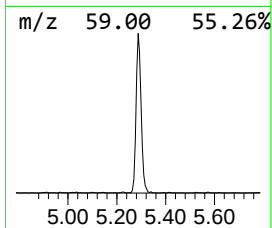
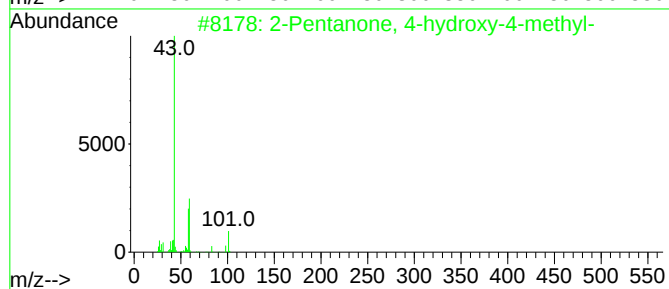
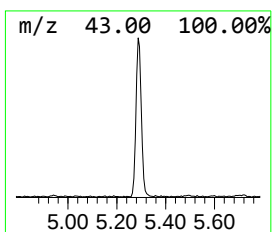
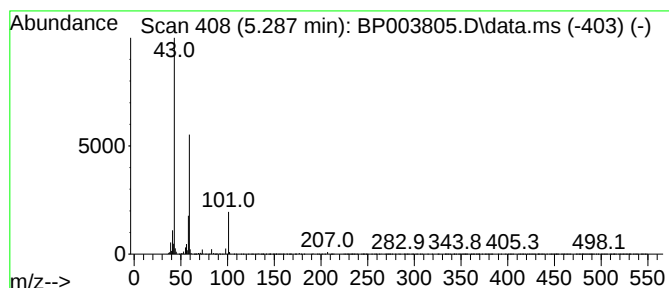
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.287	2.81 ng	105900	1,4-Dichlorobenzene-d4	8.293

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Hexanamide	115	C6H13NO	000628-02-4	17
3			2,5,8,11-Tetraoxadodecane	178	C8H18O4	000112-49-2	17
4			Butane	58	C4H10	000106-97-8	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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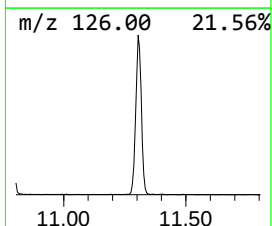
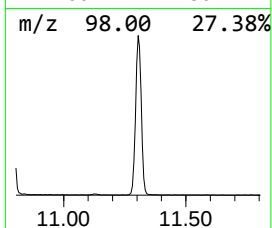
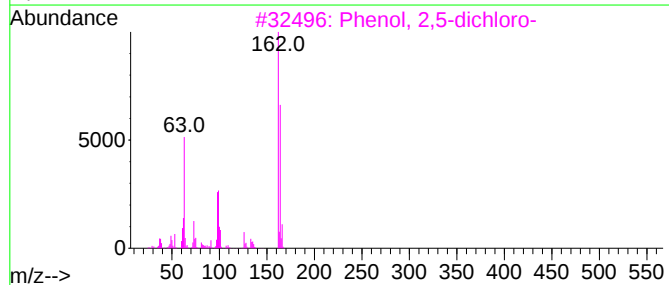
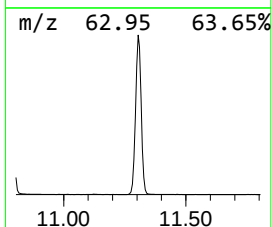
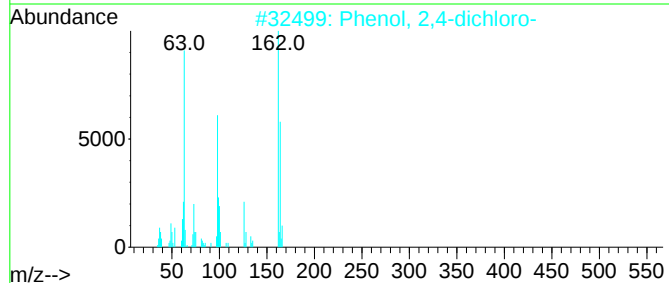
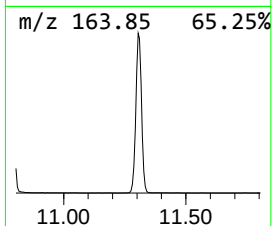
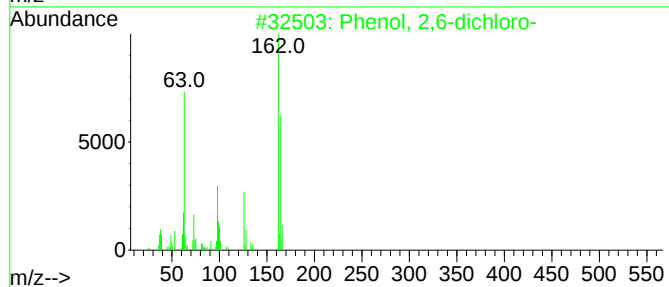
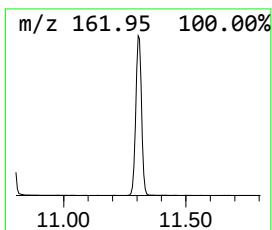
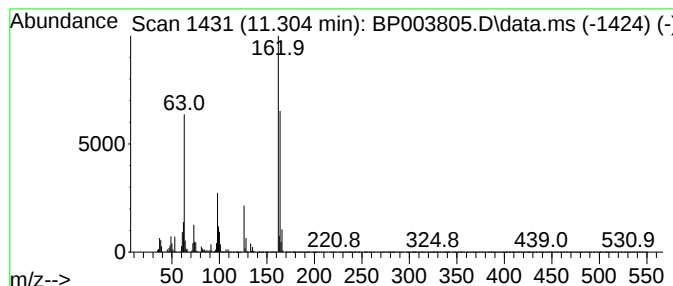
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Phenol, 2,6-dichloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.304	42.68 ng	2125950	Naphthalene-d8	11.128

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2,6-dichloro-	162	C6H4Cl2O	000087-65-0	98
2			Phenol, 2,4-dichloro-	162	C6H4Cl2O	000120-83-2	97
3			Phenol, 2,5-dichloro-	162	C6H4Cl2O	000583-78-8	94
4			Phenol, 2,3-dichloro-	162	C6H4Cl2O	000576-24-9	94
5			Phenol, 3,5-dichloro-	162	C6H4Cl2O	000591-35-5	50



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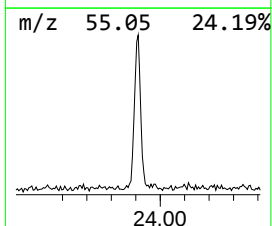
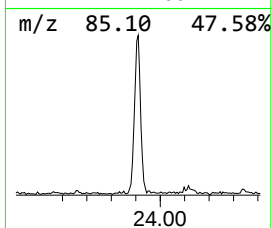
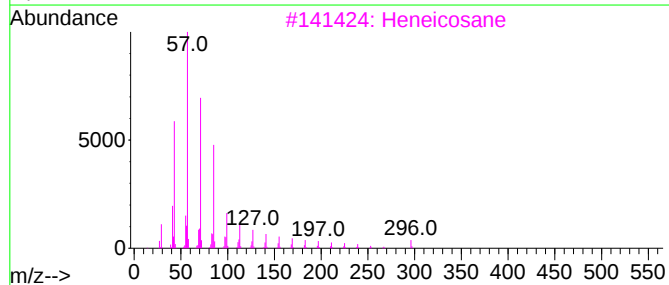
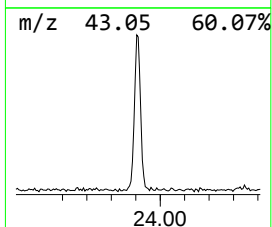
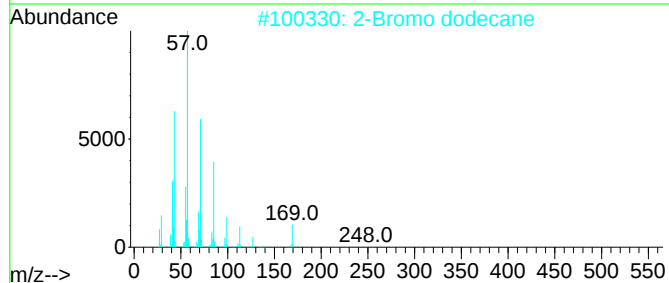
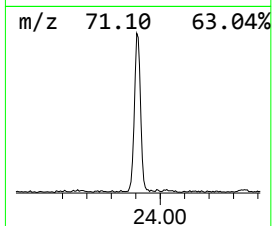
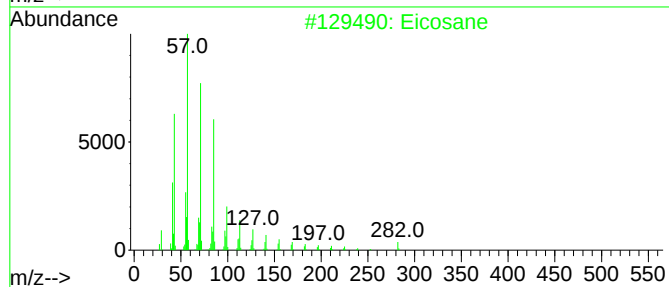
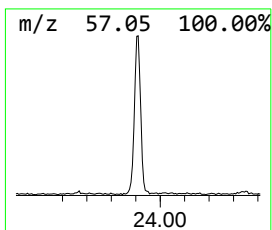
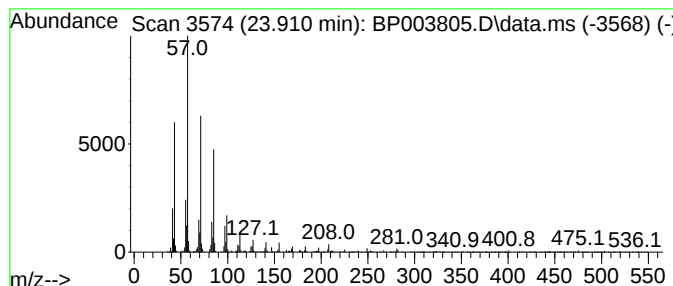
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Eicosane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.910	3.05 ng	229948	Perylene-d12	24.121

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	96
2			2-Bromo dodecane	248	C12H25Br	013187-99-0	93
3			Heneicosane	296	C21H44	000629-94-7	91
4			Octacosane	394	C28H58	000630-02-4	90
5			Tetratetracontane	619	C44H90	007098-22-8	90



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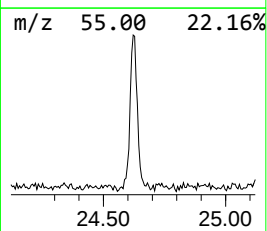
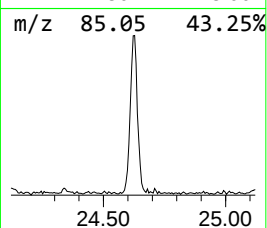
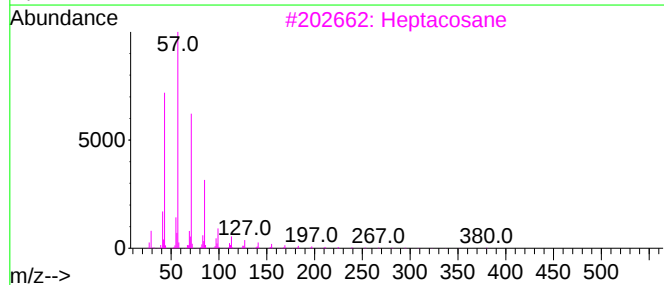
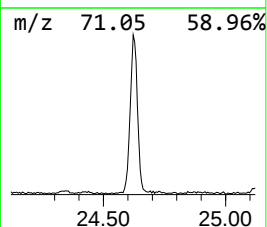
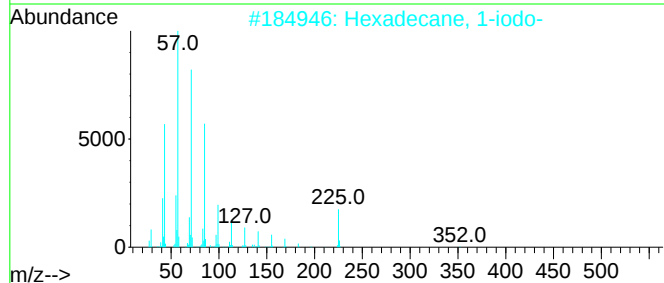
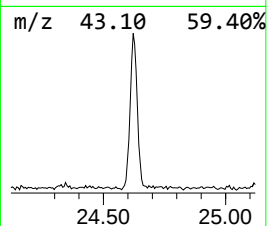
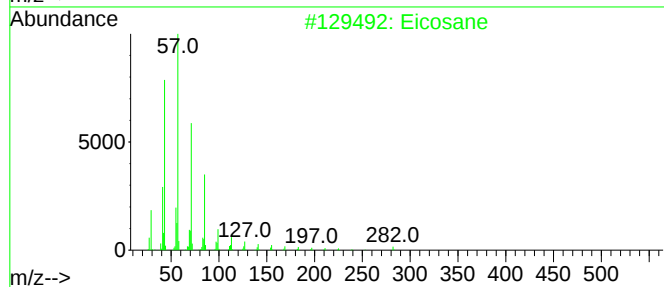
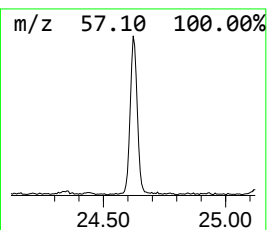
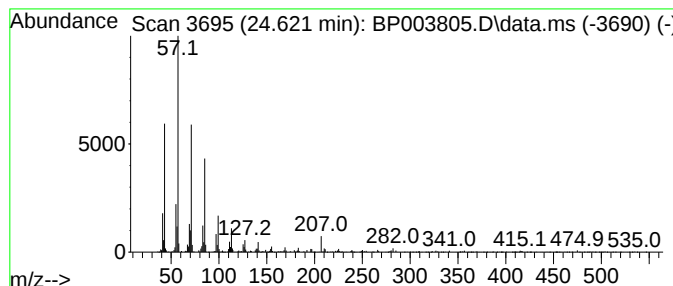
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Hexadecane, 1-iodo- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
24.621	3.11 ng	234315	Perylene-d12	24.121	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Eicosane	282	C20H42	000112-95-8	92
2	Hexadecane, 1-iodo-	352	C16H33I	000544-77-4	90
3	Heptacosane	380	C27H56	000593-49-7	90
4	Tetracosane	338	C24H50	000646-31-1	90
5	Octacosane	394	C28H58	000630-02-4	90



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ClientSampleId :
PT-ACIDS-WP

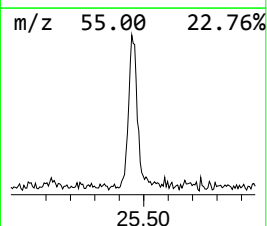
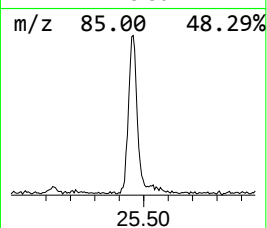
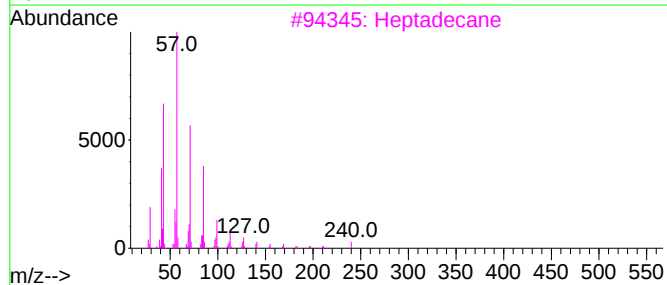
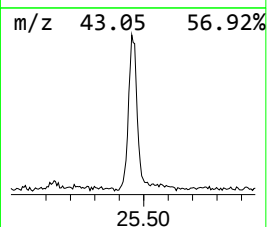
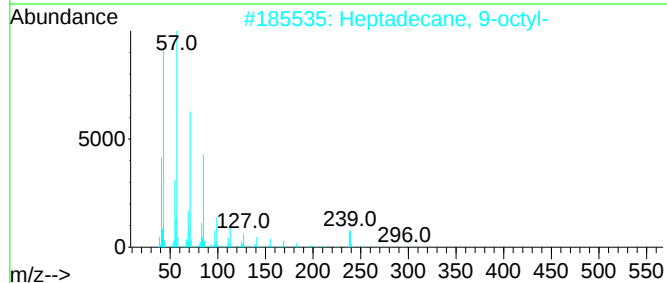
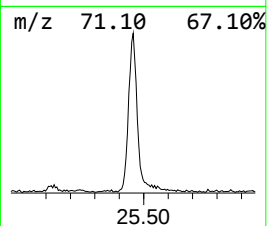
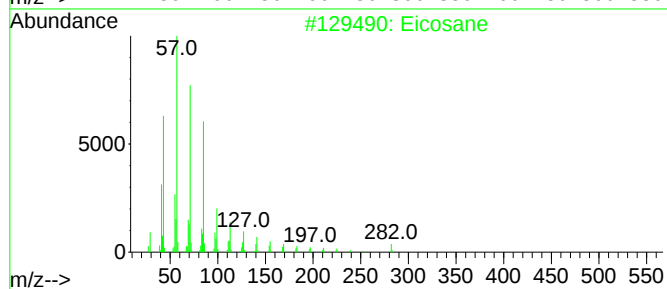
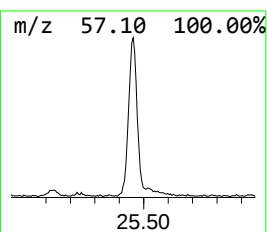
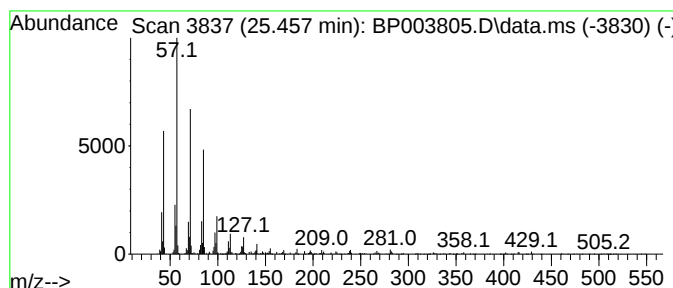
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Heptadecane, 9-octyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.457	3.17 ng	238883	Perylene-d12	24.121

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Eicosane	282	C20H42	000112-95-8	95
2			Heptadecane, 9-octyl-	352	C25H52	007225-64-1	93
3			Heptadecane	240	C17H36	000629-78-7	93
4			Hexacosane	366	C26H54	000630-01-3	90
5			Heneicosane	296	C21H44	000629-94-7	90



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110420\
Data File : BP003805.D
Acq On : 04 Nov 2020 14:28
Operator : CG/JU
Sample : L3971-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PT-ACIDS-WP

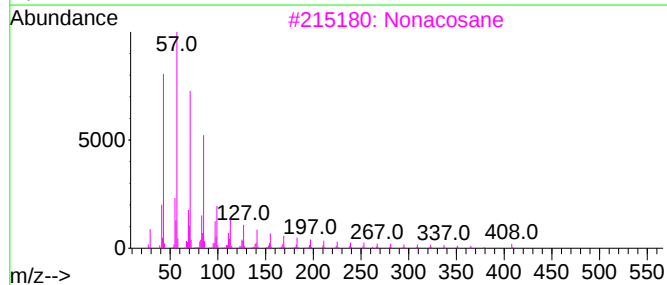
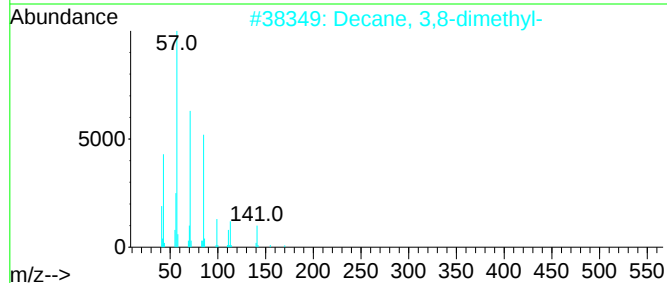
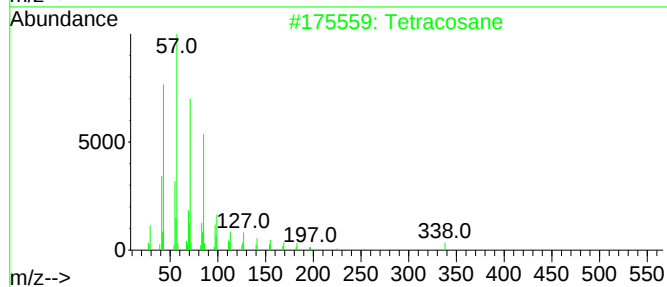
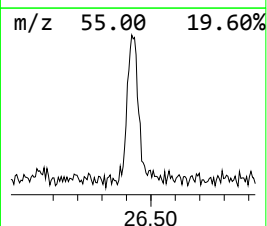
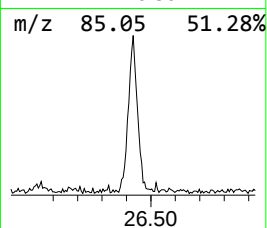
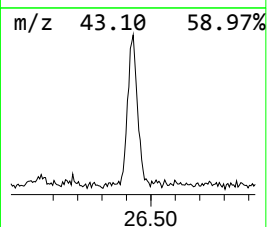
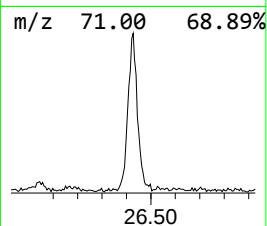
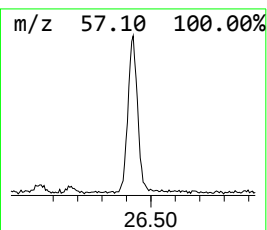
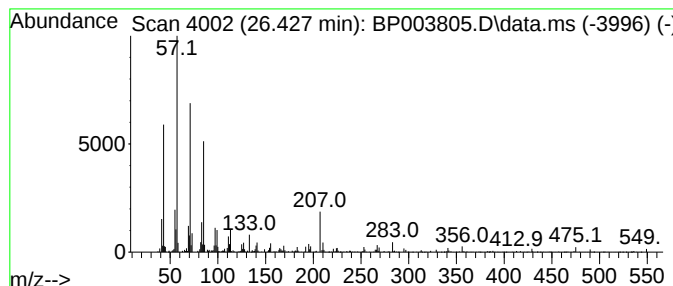
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Tetracosane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.427	2.36 ng	177425	Perylene-d12	24.121

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Tetracosane	338	C24H50	000646-31-1	89
2			Decane, 3,8-dimethyl-	170	C12H26	017312-55-9	76
3			Nonacosane	408	C29H60	000630-03-5	76
4			Decane, 1-iodo-	268	C10H21I	002050-77-3	64
5			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	64



Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP110420\
Data File : BP003805.D
Acq On : 04 Nov 2020 14:28
Operator : CG/JU
Sample : L3971-06
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
PT-ACIDS-WP

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_P\METHODS\8270-BP110320.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...	3.193	9.8	ng	368694	1	8.293	754098	20.0
2-Pentanone, 4-...	5.287	2.8	ng	105900	1	8.293	754098	20.0
Phenol, 2,6-dic...	11.304	42.7	ng	2125950	2	11.128	996277	20.0
Eicosane	23.910	3.0	ng	229948	6	24.121	1506720	20.0
Hexadecane, 1-i...	24.621	3.1	ng	234315	6	24.121	1506720	20.0
Heptadecane, 9-...	25.457	3.2	ng	238883	6	24.121	1506720	20.0
Tetracosane	26.427	2.4	ng	177425	6	24.121	1506720	20.0