

Data Path : Z:\HPCHEM1\BNA F\DATA\BF042718\
 Data File : BF104898.D
 Acq On : 27 Apr 2018 22:53
 Operator : JU/SJ
 Sample : J2549-13
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.022	495	499	509	rBV	92339	136787	4.43%	0.523%
2	5.422	563	567	581	rBV	2535550	2914463	94.34%	11.148%
3	6.451	736	742	758	rBV	2473958	3089393	100.00%	11.818%
4	6.575	758	763	766	rBV	3026980	2982866	96.55%	11.410%
5	6.798	798	801	805	rBV	801628	630283	20.40%	2.411%
6	6.957	823	828	831	rBV	2655038	2327016	75.32%	8.901%
7	7.369	893	898	901	rBV	1836846	1802086	58.33%	6.893%
8	8.081	1016	1019	1039	rVB	781825	807570	26.14%	3.089%
9	9.157	1198	1202	1212	rBV	2971205	2944028	95.29%	11.262%
10	9.551	1265	1269	1277	rBV	338030	306113	9.91%	1.171%
11	9.763	1301	1305	1309	rBV	50524	42406	1.37%	0.162%
12	9.839	1314	1318	1322	rBV	937167	791277	25.61%	3.027%
13	10.257	1387	1389	1392	rVB	62192	52545	1.70%	0.201%
14	10.633	1449	1453	1462	rBV	1726811	1715998	55.54%	6.564%
15	10.733	1467	1470	1475	rVV	57697	55994	1.81%	0.214%
16	11.333	1568	1572	1574	rBV	743802	704022	22.79%	2.693%
17	11.351	1574	1575	1581	rVV	168631	151507	4.90%	0.580%
18	11.410	1581	1585	1590	rVB	39749	42067	1.36%	0.161%
19	11.851	1656	1660	1668	rBV2	213526	234103	7.58%	0.895%
20	12.545	1775	1778	1783	rBV	202325	189961	6.15%	0.727%
21	12.639	1791	1794	1800	rBV3	44011	53422	1.73%	0.204%
22	12.780	1812	1818	1824	rBV	170683	203269	6.58%	0.778%
23	12.851	1827	1830	1835	rVB	67621	57827	1.87%	0.221%
24	12.922	1837	1842	1845	rBV	2455486	2279095	73.77%	8.718%
25	13.192	1886	1888	1891	rBV	97067	74570	2.41%	0.285%
26	13.804	1989	1992	1995	rBV3	84674	75953	2.46%	0.291%
27	13.839	1996	1998	2003	rVB	55243	59324	1.92%	0.227%
28	13.980	2017	2022	2025	rBV	705300	724983	23.47%	2.773%
29	14.004	2025	2026	2033	rVB	85431	61861	2.00%	0.237%
30	15.021	2196	2199	2202	rBV	51504	66532	2.15%	0.254%
31	15.380	2258	2260	2267	rVB	37933	48689	1.58%	0.186%
32	15.451	2267	2272	2281	rVB	367025	516404	16.72%	1.975%

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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

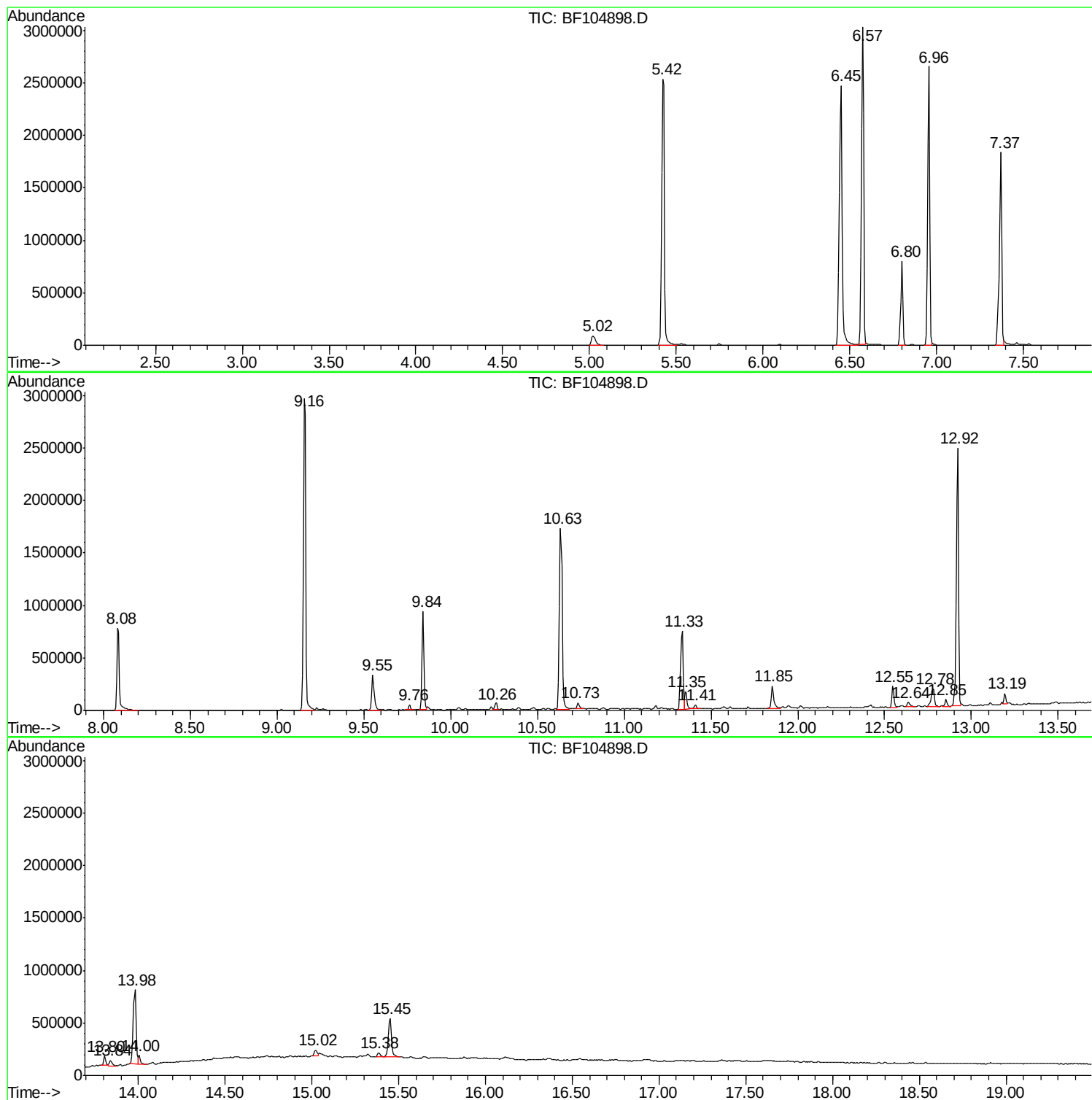
Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Sum of corrected areas: 26142414

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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF040618.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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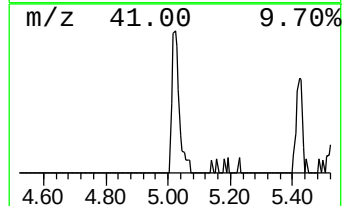
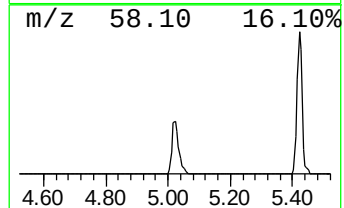
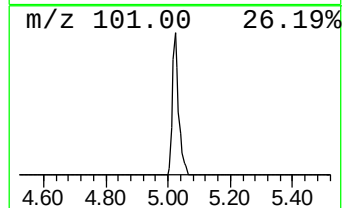
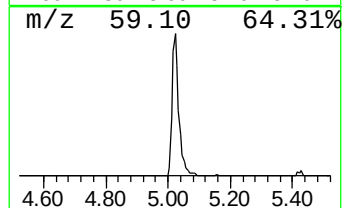
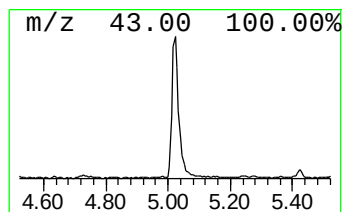
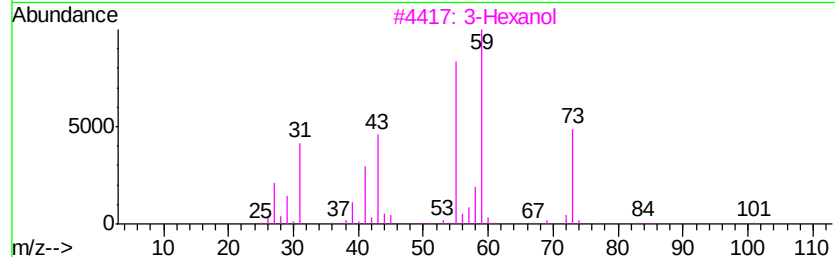
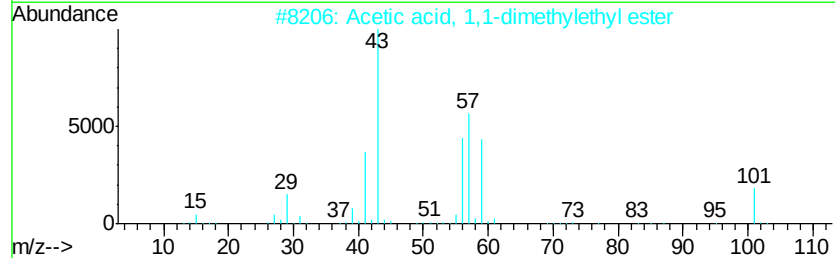
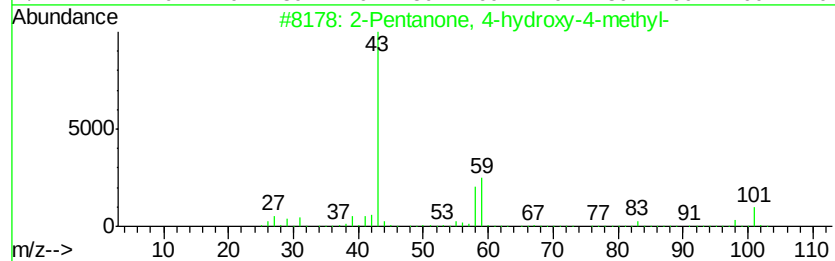
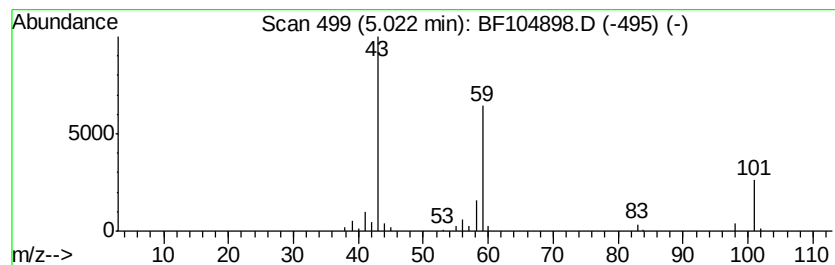
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.02	4.34 ng	136787	1,4-Dichlorobenzene-d4	6.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3			3-Hexanol	102	C6H14O	000623-37-0	25
4			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	16



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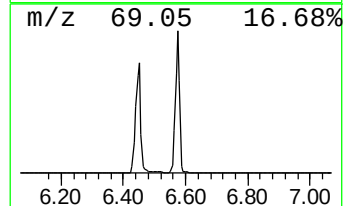
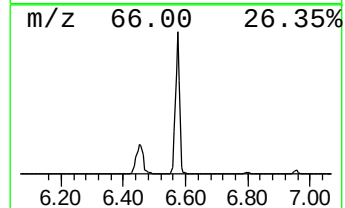
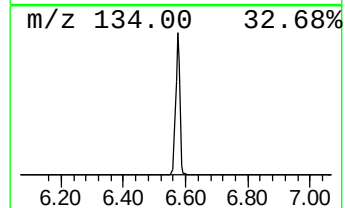
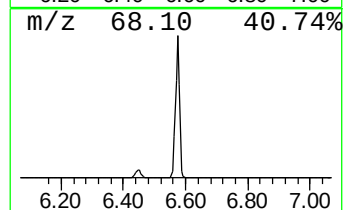
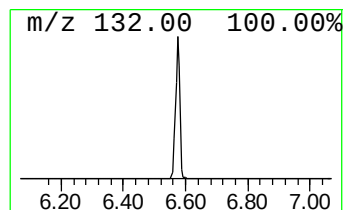
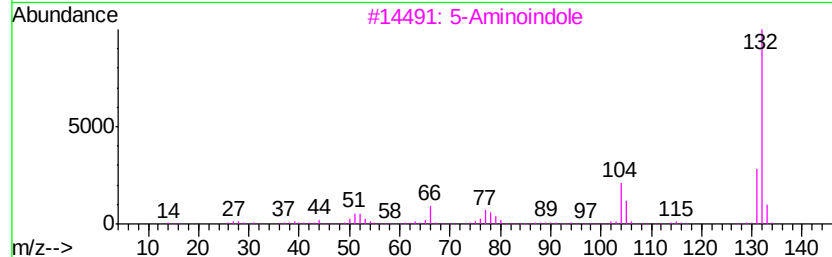
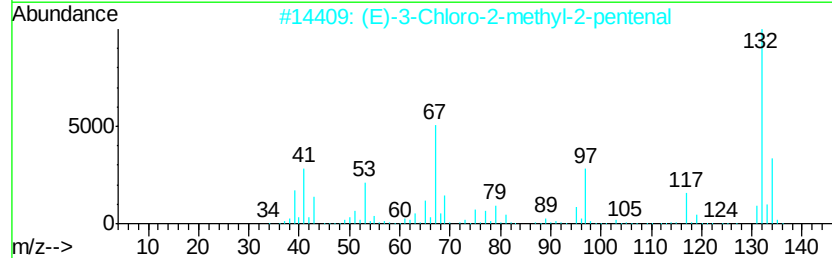
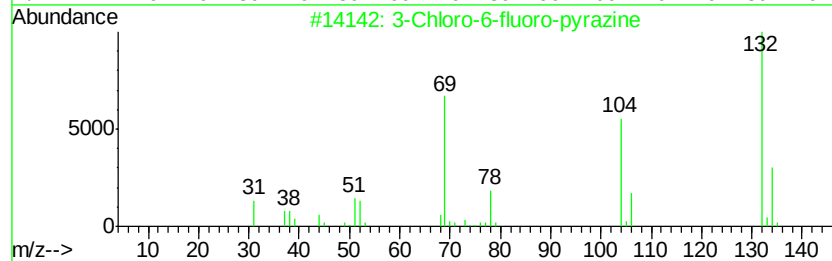
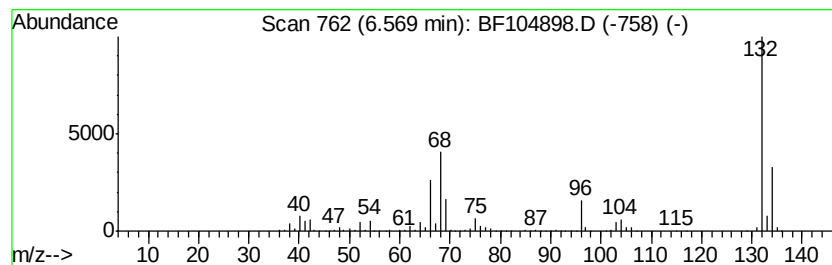
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Peak Number 2 unknown6.57 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.57	94.65 ng	2982870	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



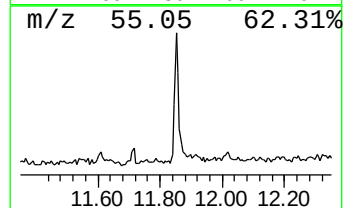
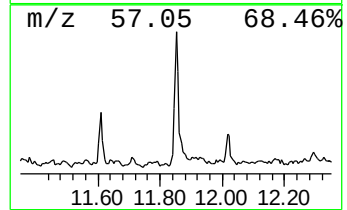
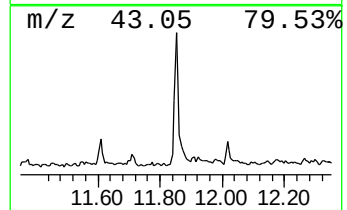
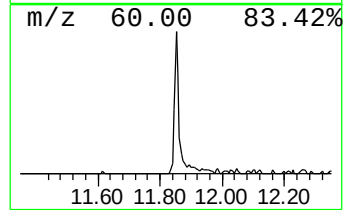
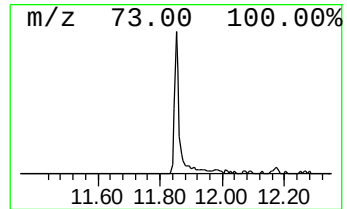
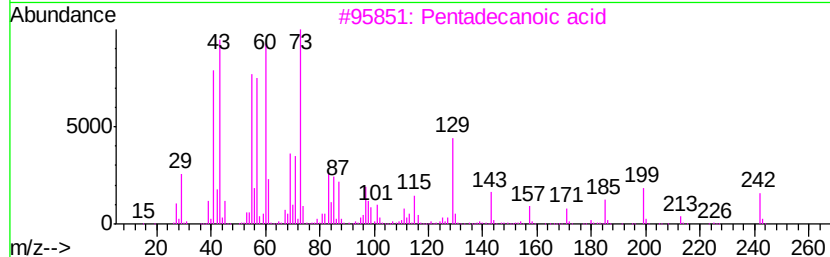
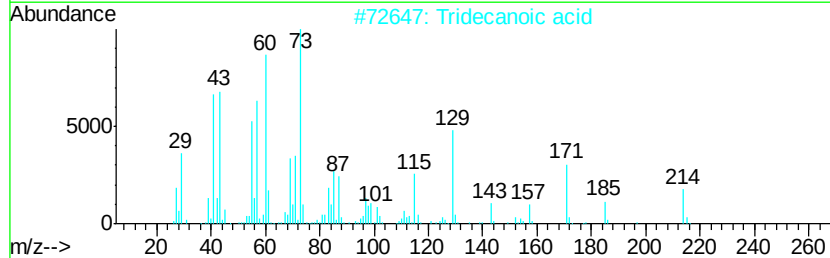
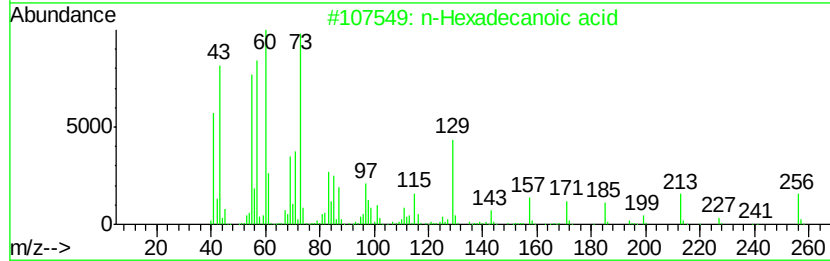
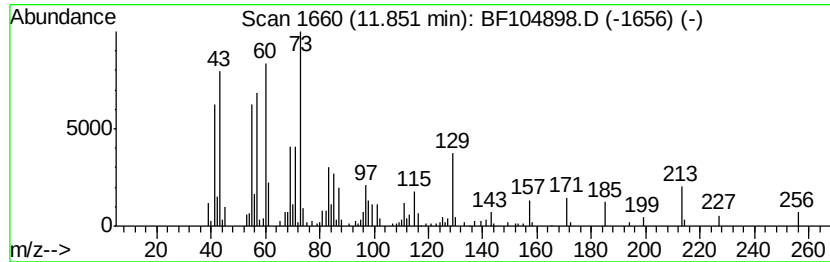
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.85	6.65 ng	234103	Phenanthrene-d10		11.33
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	95
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	90
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5	n-Decanoic acid	172	C10H20O2	000334-48-5	53



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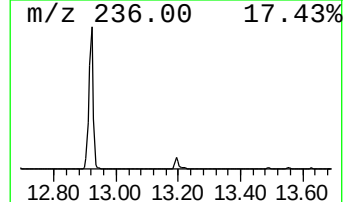
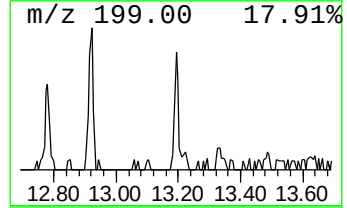
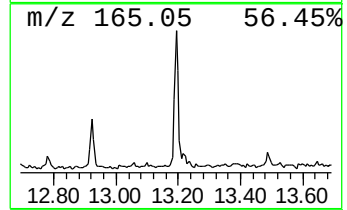
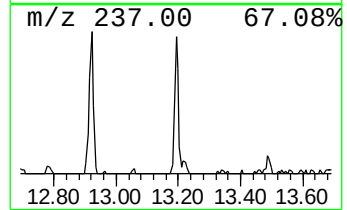
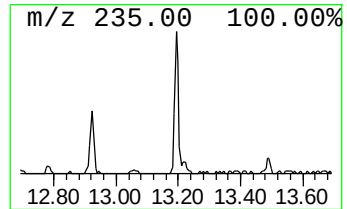
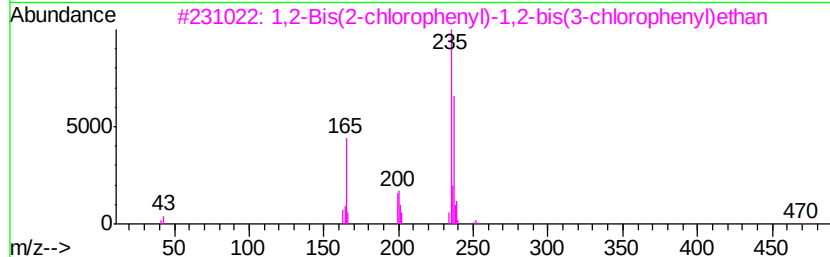
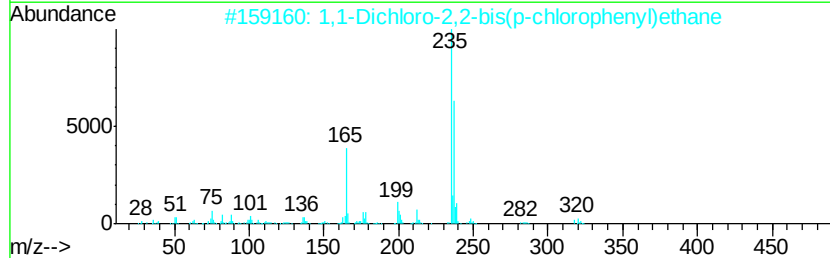
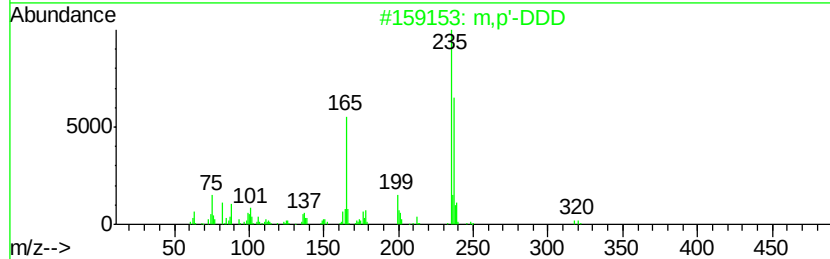
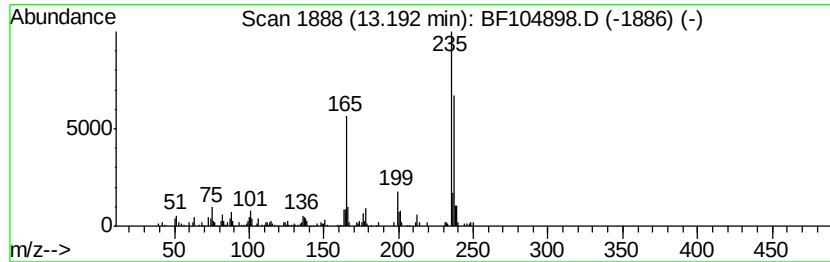
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 m,p'-DDD Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.19	2.06 ng	74570	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	m,p'-DDD	318	C14H10Cl4	004329-12-8	91
2		1,1-Dichloro-2,2-bis(p-chlorophe...	318	C14H10Cl4	000072-54-8	87
3		1,2-Bis(2-chlorophenyl)-1,2-bis(...	470	C26H18Cl4	1000137-94-8	80
4		3-Butanone, 1,1-bis(4-chlorophen...	320	C18H18Cl2O	1000158-20-4	80
5		Benzene, 1-methoxy-4-(2-cyano-2-...	235	C16H13NO	005432-07-5	52



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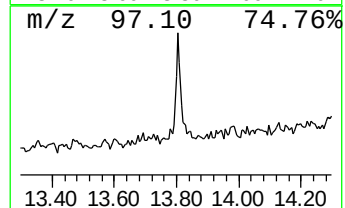
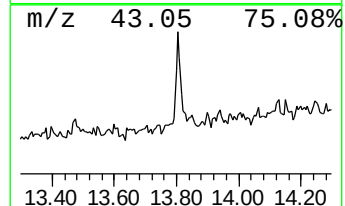
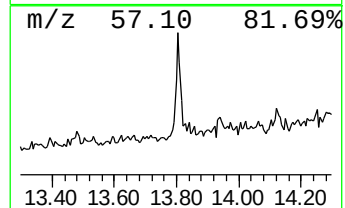
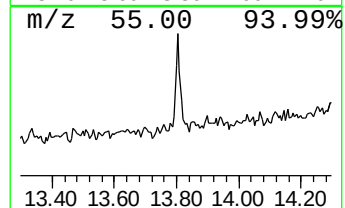
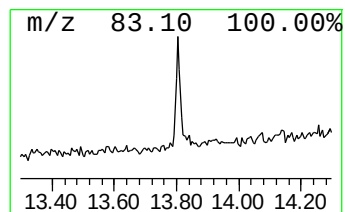
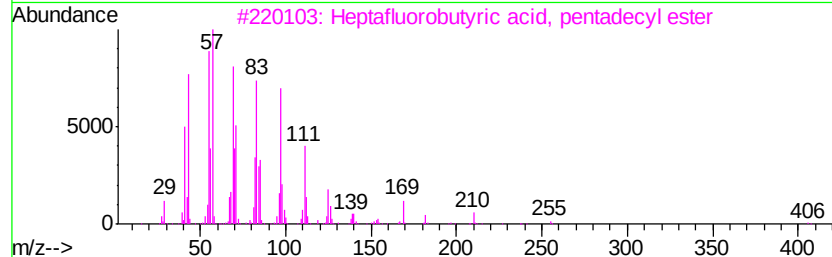
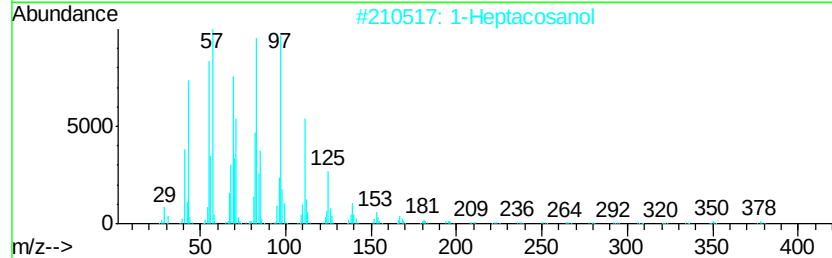
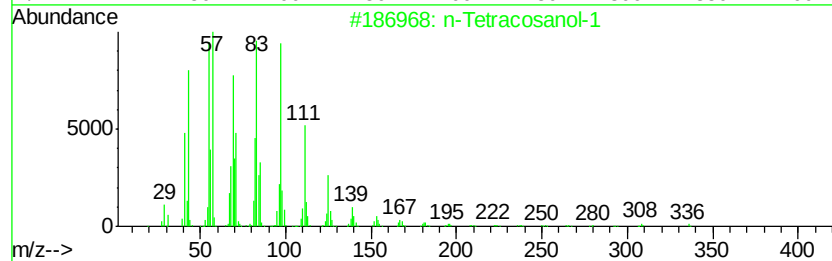
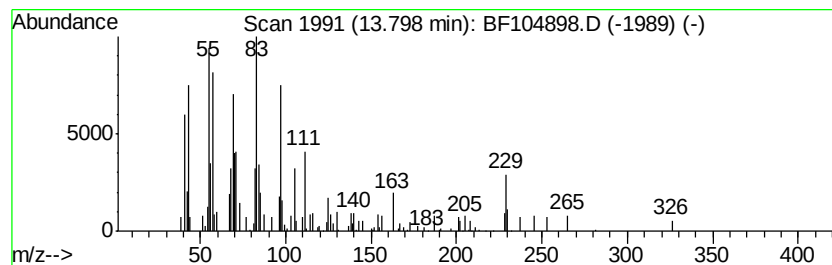
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 n-Tetracosanol-1 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.80	2.10 ng	75953	Chrysene-d12	13.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93
2		1-Heptacosanol	396	C27H56O	002004-39-9	93
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
4		1-Heneicosyl formate	340	C22H44O2	077899-03-7	93
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.02	4.3	ng	136787	1	6.80	630283	20.0
unknown6.57	6.57	94.7	ng	2982870	1	6.80	630283	20.0
n-Hexadecanoic acid	11.85	6.7	ng	234103	4	11.33	704022	20.0
m,p'-DDD	13.19	2.1	ng	74570	5	13.98	724983	20.0
n-Tetracosanol-1	13.80	2.1	ng	75953	5	13.98	724983	20.0