

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
 Data File : BF126251.D
 Acq On : 18 Dec 2021 13:34
 Operator : JU/CG
 Sample : M5081-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CONCRETE

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-BF121521.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF126251.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	724250	839522	18.29%	2.452%
2	2.222	19	23	30	rVB	75534	105530	2.30%	0.308%
3	3.887	302	306	314	rVB	37036	54981	1.20%	0.161%
4	4.404	390	394	400	rVB	49848	55053	1.20%	0.161%
5	5.022	494	499	503	rBV	1509731	1697769	36.99%	4.958%
6	5.428	561	568	571	rBV	2147673	2100813	45.78%	6.135%
7	5.828	633	636	641	rBV	88692	70652	1.54%	0.206%
8	6.440	734	740	743	rBV	3635554	3808628	82.99%	11.123%
9	6.640	772	774	780	rBV2	64372	82486	1.80%	0.241%
10	6.816	800	804	807	rBV	1619698	1332518	29.04%	3.892%
11	6.881	811	815	822	rBV	44851	59410	1.29%	0.174%
12	7.216	865	872	876	rBV2	62569	67851	1.48%	0.198%
13	7.375	893	899	902	rBV	2963742	3016793	65.74%	8.811%
14	8.004	1002	1006	1013	rBV	111156	158263	3.45%	0.462%
15	8.098	1017	1022	1025	rBV	2130409	1888859	41.16%	5.516%
16	9.175	1200	1205	1209	rBV	4401723	4589190	100.00%	13.403%
17	9.263	1216	1220	1224	rBV2	121336	111419	2.43%	0.325%
18	9.675	1286	1290	1299	rBV5	66102	150460	3.28%	0.439%
19	9.792	1307	1310	1312	rVB	84615	63869	1.39%	0.187%
20	9.851	1316	1320	1327	rVV	2204650	1979814	43.14%	5.782%
21	10.263	1387	1390	1393	rBV2	228360	202049	4.40%	0.590%
22	10.292	1393	1395	1398	rVB	106073	80124	1.75%	0.234%
23	10.563	1437	1441	1444	rBV	146758	128696	2.80%	0.376%
24	10.633	1450	1453	1457	rVB2	57644	50561	1.10%	0.148%
25	10.716	1457	1467	1469	rBV6	38733	92623	2.02%	0.271%
26	10.763	1472	1475	1480	rVB	85118	85884	1.87%	0.251%
27	10.857	1488	1491	1496	rVB2	45908	47650	1.04%	0.139%
28	11.045	1520	1523	1528	rVB4	64111	52825	1.15%	0.154%
29	11.210	1548	1551	1555	rBV2	104682	91187	1.99%	0.266%
30	11.304	1562	1567	1569	rBV	188694	181036	3.94%	0.529%
31	11.333	1569	1572	1576	rVV	2089210	1945767	42.40%	5.683%
32	11.392	1579	1582	1586	rVB4	43862	57586	1.25%	0.168%
33	11.504	1598	1601	1608	rVB	261935	247435	5.39%	0.723%
34	11.592	1613	1616	1621	rVV5	27662	50294	1.10%	0.147%
35	11.639	1621	1624	1630	rVB2	71032	74887	1.63%	0.219%
36	11.733	1637	1640	1644	rVB	92544	87479	1.91%	0.255%

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Start Thrs: 0.2

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Stop Thrs : 0

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

Peak separation: 5

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37	11.904	1665	1669	1672	rVB	209664	179598	3.91%	0.525%
38	12.045	1691	1693	1697	rBV	81665	70794	1.54%	0.207%
39	12.122	1703	1706	1715	rBV5	80506	141233	3.08%	0.412%
40	12.322	1737	1740	1743	rBV2	65371	68063	1.48%	0.199%
41	12.380	1747	1750	1754	rBV2	46280	52402	1.14%	0.153%
42	12.433	1757	1759	1763	rVB	53573	55260	1.20%	0.161%
43	12.574	1780	1783	1785	rBV4	41570	46900	1.02%	0.137%
44	12.927	1838	1843	1846	rBV	4150247	4217251	91.90%	12.316%
45	13.545	1945	1948	1951	rVB	52930	46974	1.02%	0.137%
46	13.621	1958	1961	1967	rVB3	42910	51976	1.13%	0.152%
47	13.774	1984	1987	1991	rVB	41127	46507	1.01%	0.136%
48	13.816	1991	1994	1995	rBV	55756	53963	1.18%	0.158%
49	13.851	1995	2000	2012	rVV5	190498	576445	12.56%	1.684%
50	13.968	2016	2020	2024	rVV	1544427	1497538	32.63%	4.374%
51	14.451	2099	2102	2105	rBV	47083	51335	1.12%	0.150%
52	14.833	2163	2167	2170	rBV	93359	89257	1.94%	0.261%
53	15.415	2261	2266	2272	rBV	935245	1236445	26.94%	3.611%
54	15.898	2344	2348	2356	rVB2	31769	48835	1.06%	0.143%

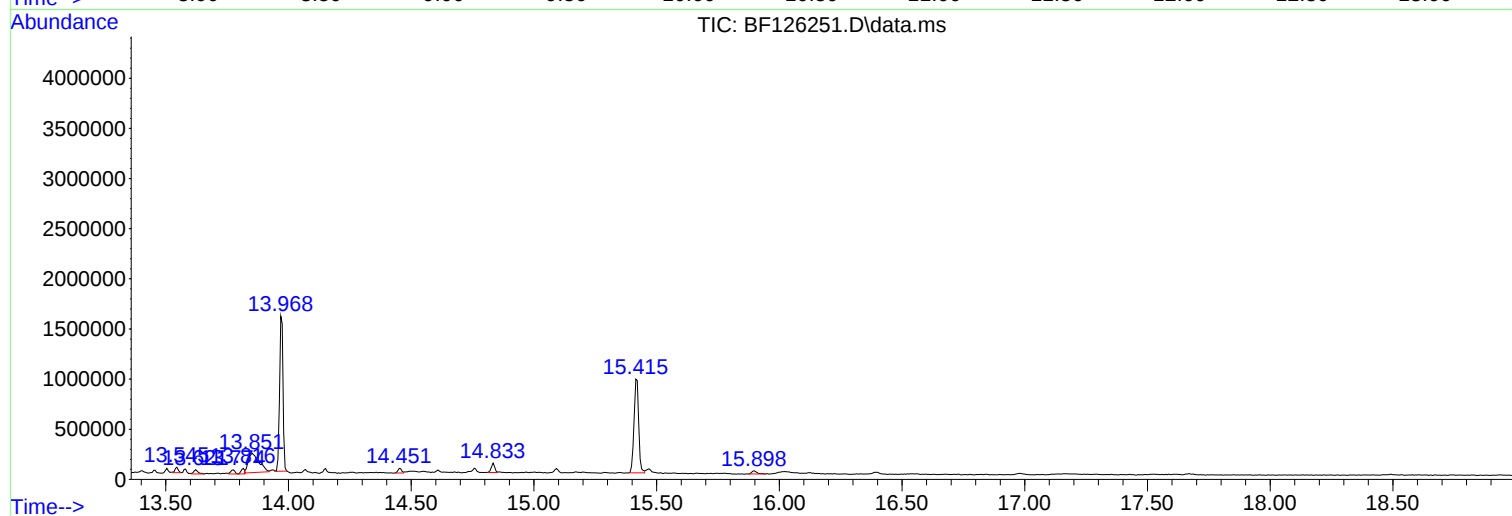
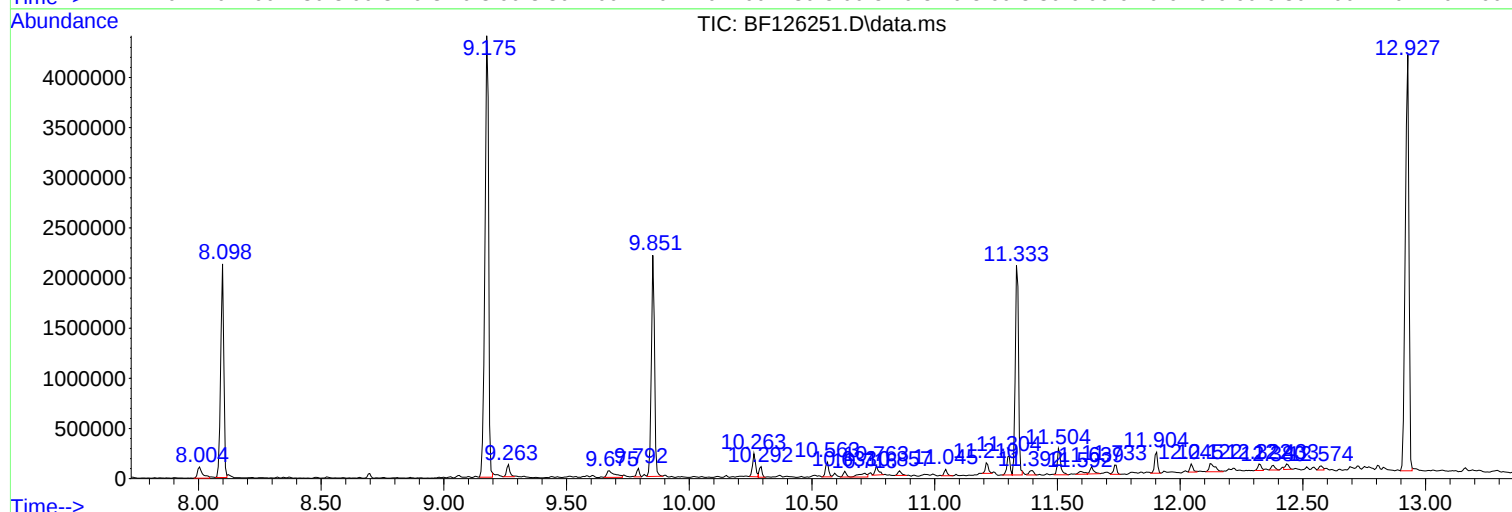
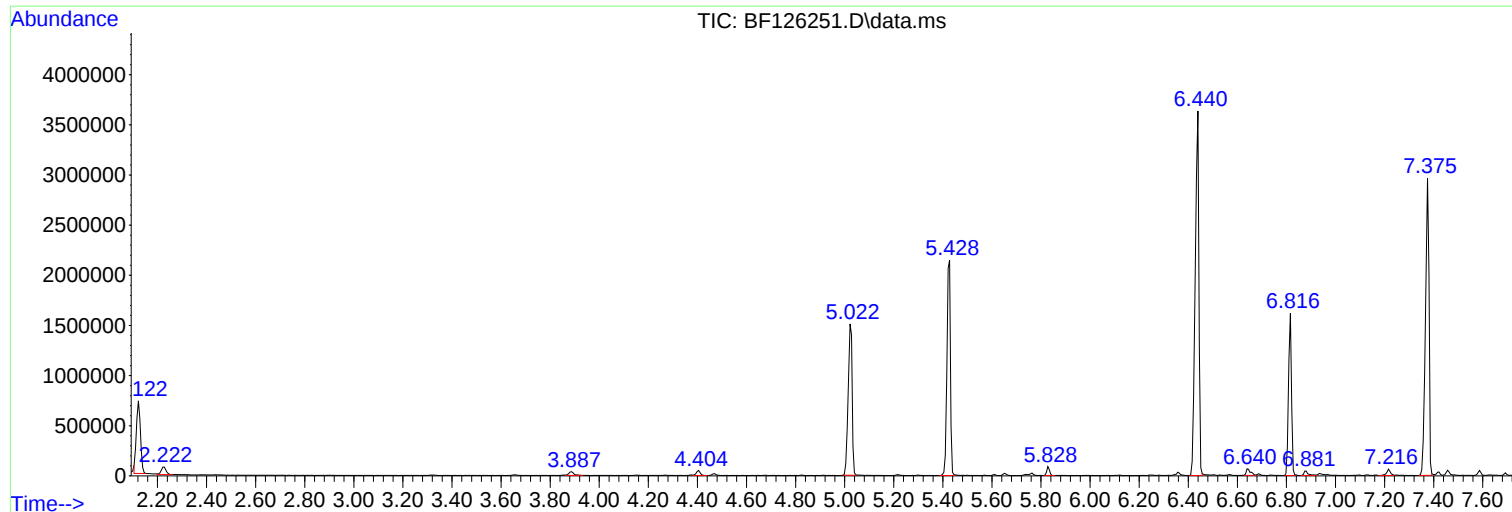
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Operator : JU/CG
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Instrument :
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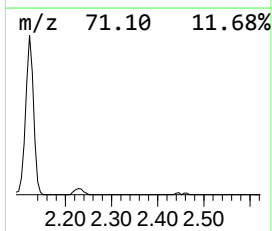
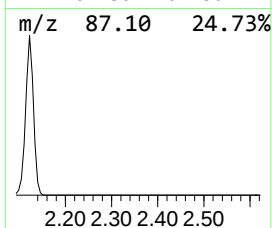
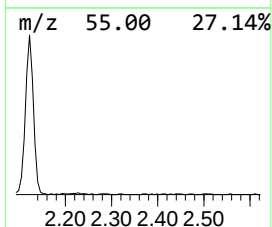
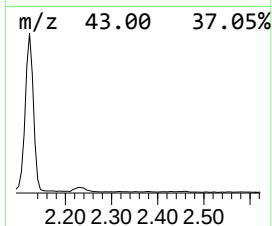
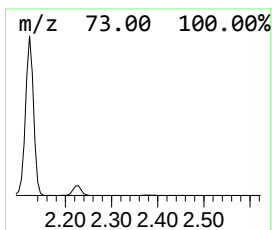
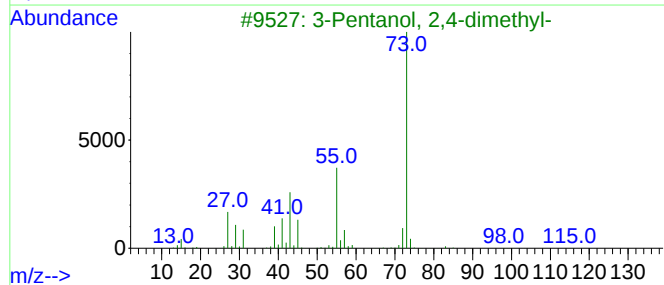
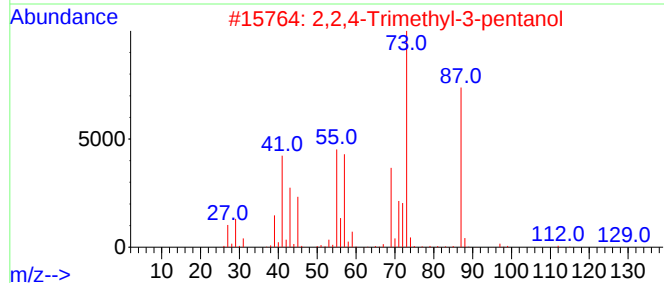
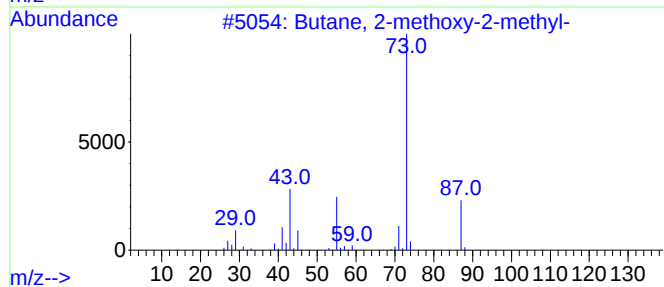
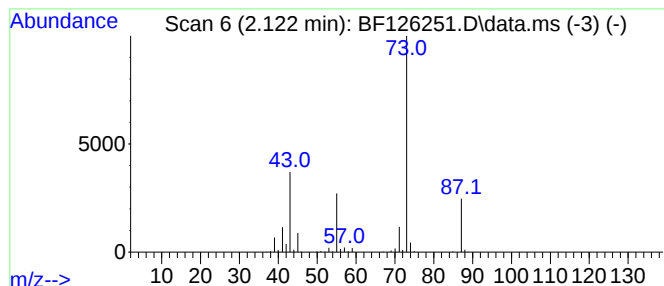
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.122	12.60 ng	839522	1,4-Dichlorobenzene-d4	6.816

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			3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	32
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23



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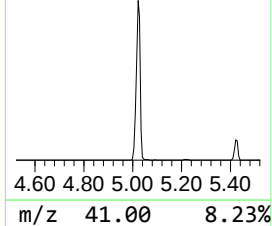
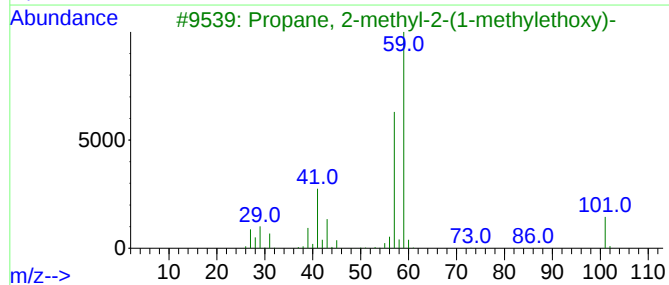
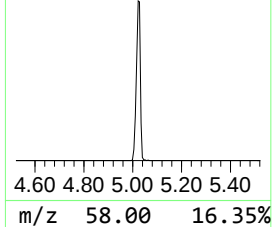
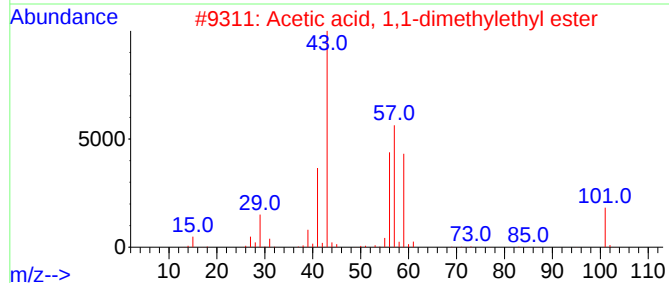
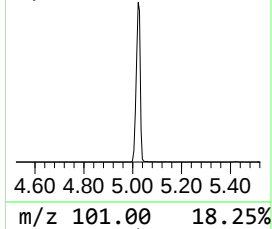
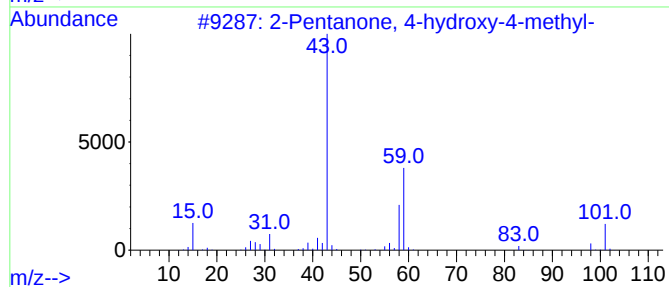
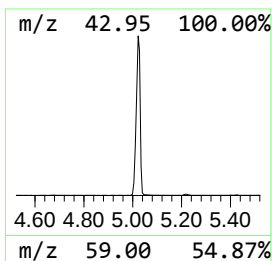
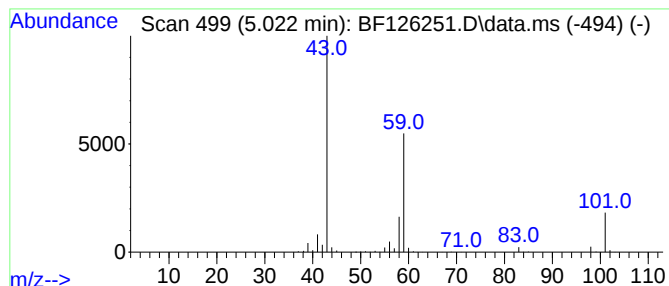
Instrument :
BNA_F
ClientSampleId :
CONCRETE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.022	25.48 ng	1697770	1,4-Dichlorobenzene-d4	6.816	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	38
3	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33
4	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5	Acetone	58	C3H6O	000067-64-1	9



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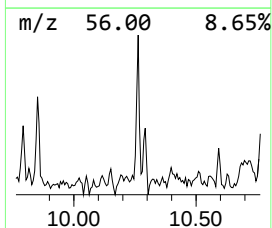
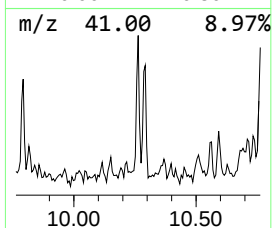
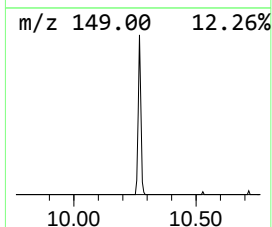
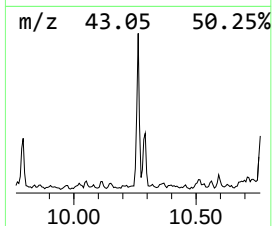
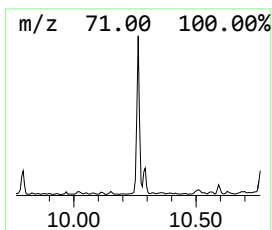
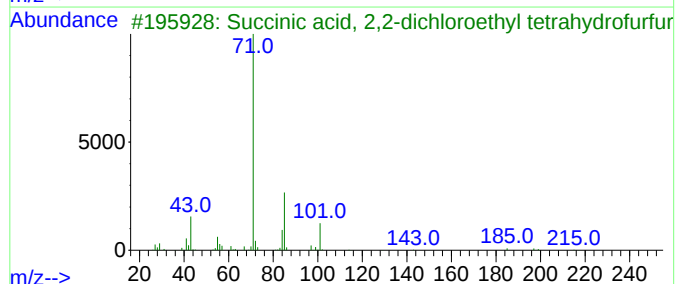
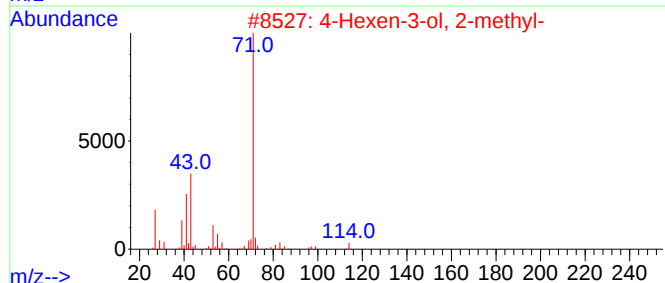
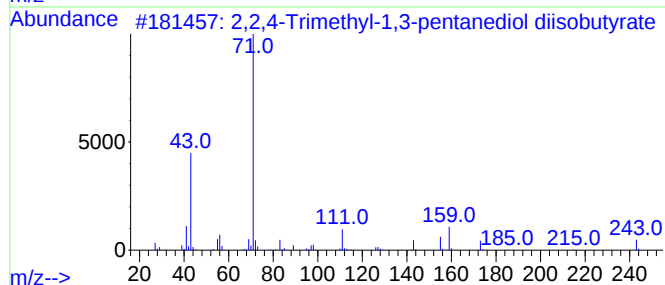
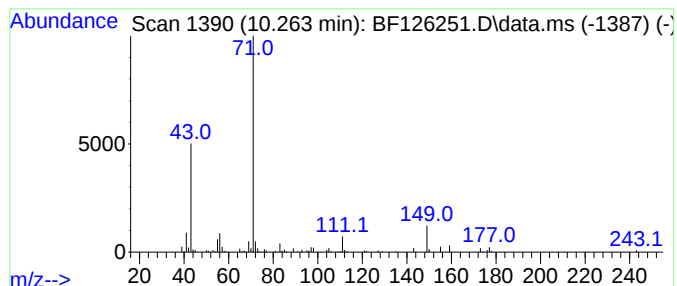
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TIC Library : C:\Database\NIST20.L
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Peak Number 3 2,2,4-Trimethyl-1,3-pentane... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.263	2.04 ng	202049	Acenaphthene-d10	9.851

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	59
2			4-Hexen-3-ol, 2-methyl-	114	C7H14O	004798-60-1	53
3			Succinic acid, 2,2-dichloroethyl...	298	C11H16Cl2O5	1000390-71-6	53
4			Sulfurous acid, octyl 2-pentyl e...	264	C13H28O3S	1000309-15-7	45
5			Oxalic acid, decyl neopentyl ester	300	C17H32O4	1000309-73-4	45



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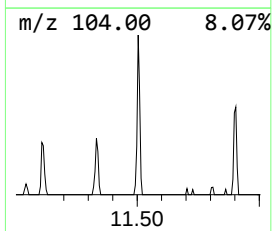
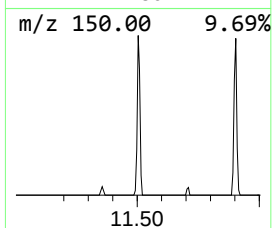
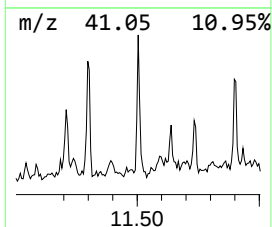
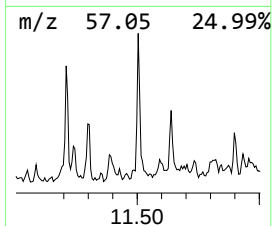
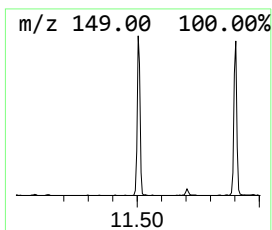
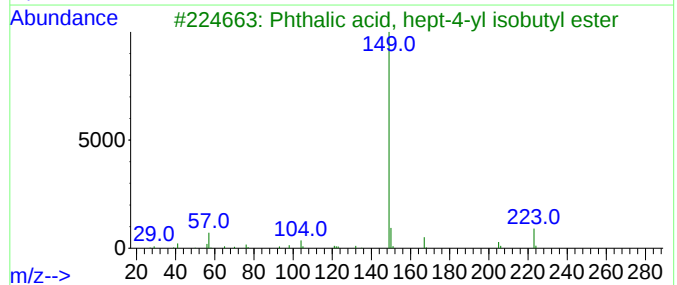
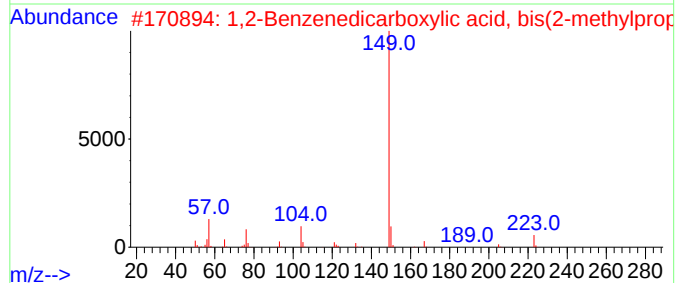
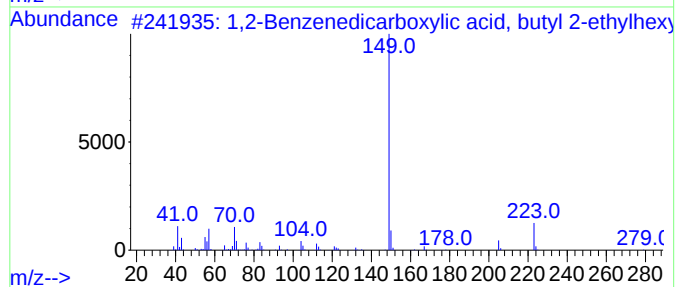
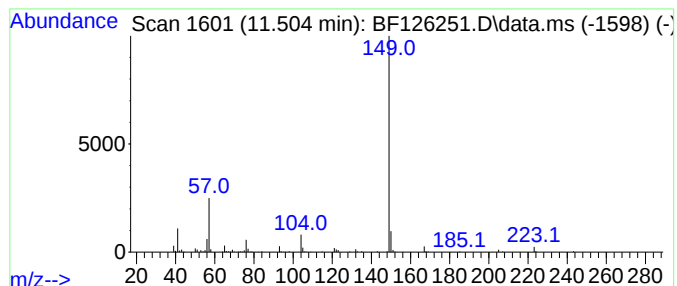
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 1,2-Benzenedicarboxylic aci... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.504	2.54 ng	247435	Phenanthrene-d10	11.333

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Benzenedicarboxylic acid, bu...	334	C20H30O4	000085-69-8	83
2			1,2-Benzenedicarboxylic acid, bi...	278	C16H22O4	000084-69-5	83
3			Phthalic acid, hept-4-yl isobuty...	320	C19H28O4	1000356-78-3	83
4			1,2-Benzenedicarboxylic acid, bu...	304	C18H24O4	000084-64-0	78
5			Phthalic acid, hex-2-yn-4-yl iso...	302	C18H22O4	1000315-19-9	78



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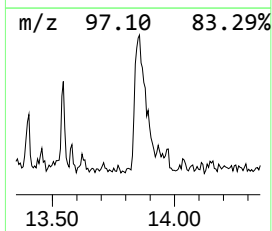
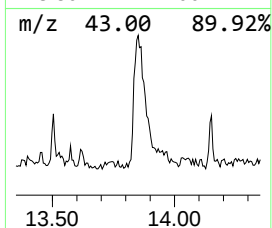
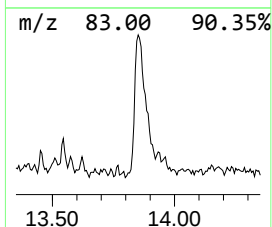
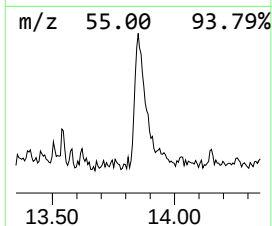
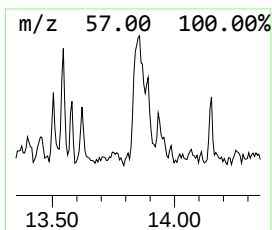
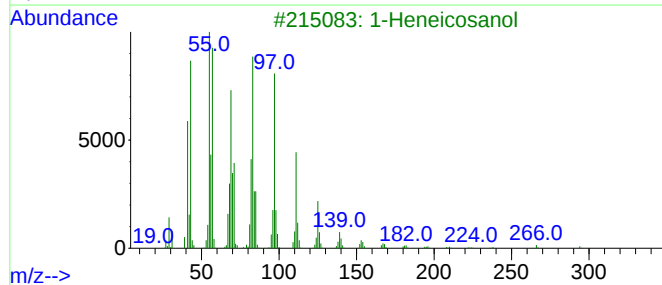
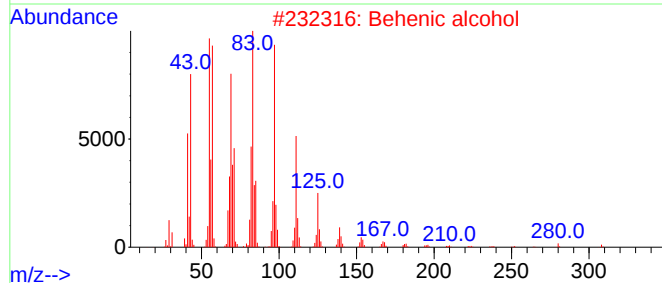
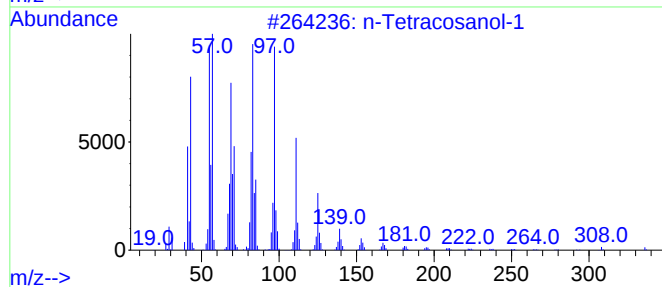
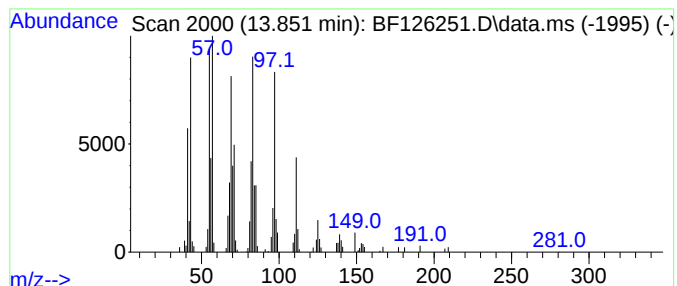
Instrument :
BNA_F
ClientSampleId :
CONCRETE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Tetracosanol-1 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.851	7.70 ng	576445	Chrysene-d12	13.974	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Tetracosanol-1	354	C24H50O	000506-51-4	94
2	Behenic alcohol	326	C22H46O	000661-19-8	94
3	1-Heneicosanol	312	C21H44O	015594-90-8	94
4	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl13O2	074339-54-1	93
5	1-Hexacosanol	382	C26H54O	000506-52-5	91



Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF121821\
Data File : BF126251.D
Acq On : 18 Dec 2021 13:34
Operator : JU/CG
Sample : M5081-01
Misc :
ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
CONCRETE

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF121521.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-metho...	2.122	12.6	ng	839522	1	6.816	1332520	20.0
2-Pentanone, 4-...	5.022	25.5	ng	1697770	1	6.816	1332520	20.0
2,2,4-Trimethyl...	10.263	2.0	ng	202049	3	9.851	1979810	20.0
1,2-Benzenedica...	11.504	2.5	ng	247435	4	11.333	1945770	20.0
n-Tetracosanol-1	13.851	7.7	ng	576445	5	13.974	1497540	20.0