

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF071023\
 Data File : BF134184.D
 Acq On : 10 Jul 2023 13:54
 Operator : CG\JU
 Sample : PB154009BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PB154009BL

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-BF062623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF134184.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.487	404	408	429	rBV	621149	697071	13.85%	2.256%
2	5.104	506	513	528	rBV	1481190	2310491	45.92%	7.476%
3	5.492	574	579	582	rBV	3413094	3424296	68.05%	11.080%
4	6.487	742	748	750	rBV	2968384	3436296	68.29%	11.119%
5	6.845	805	809	822	rBV	794054	733078	14.57%	2.372%
6	7.410	900	905	908	rBV	2404131	2286185	45.44%	7.398%
7	8.122	1022	1026	1040	rBV	1162466	998352	19.84%	3.230%
8	9.204	1205	1210	1213	rBV	4920901	4262690	84.72%	13.793%
9	9.880	1321	1325	1340	rBV	1368634	1157349	23.00%	3.745%
10	10.680	1456	1461	1464	rBV	3035761	3062031	60.85%	9.908%
11	11.374	1575	1579	1597	rBV	1407915	1293037	25.70%	4.184%
12	12.980	1847	1852	1855	rBV	5028273	5031684	100.00%	16.281%
13	14.039	2028	2032	2040	rBV	1094946	1080104	21.47%	3.495%
14	15.539	2282	2287	2299	rBV	569439	883977	17.57%	2.860%
15	16.033	2365	2371	2375	rBV2	40993	65823	1.31%	0.213%
16	16.568	2457	2462	2468	rBV	38925	70834	1.41%	0.229%
17	17.203	2565	2570	2579	rVB3	25701	53155	1.06%	0.172%
18	17.956	2694	2698	2710	rVB7	21221	58152	1.16%	0.188%

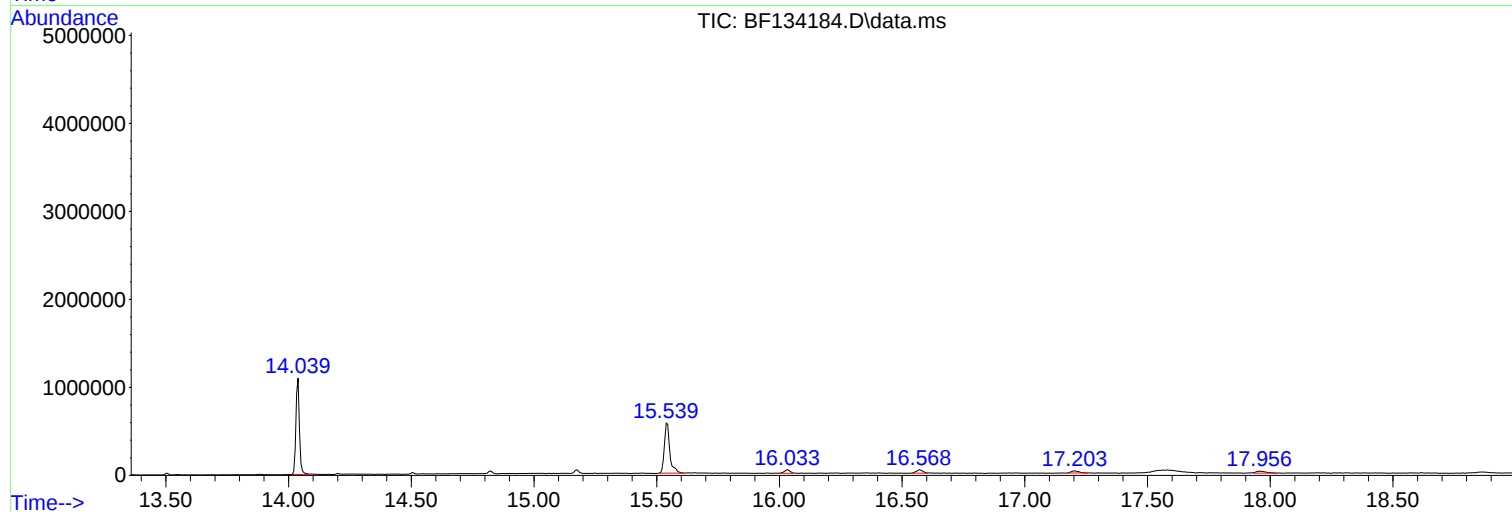
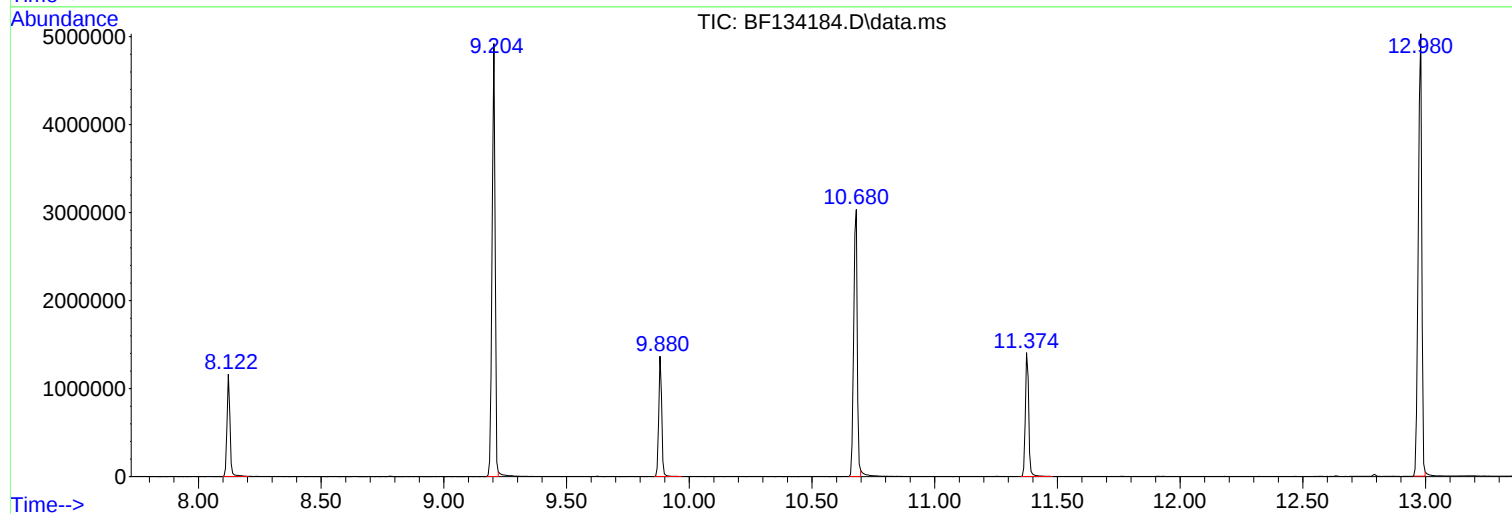
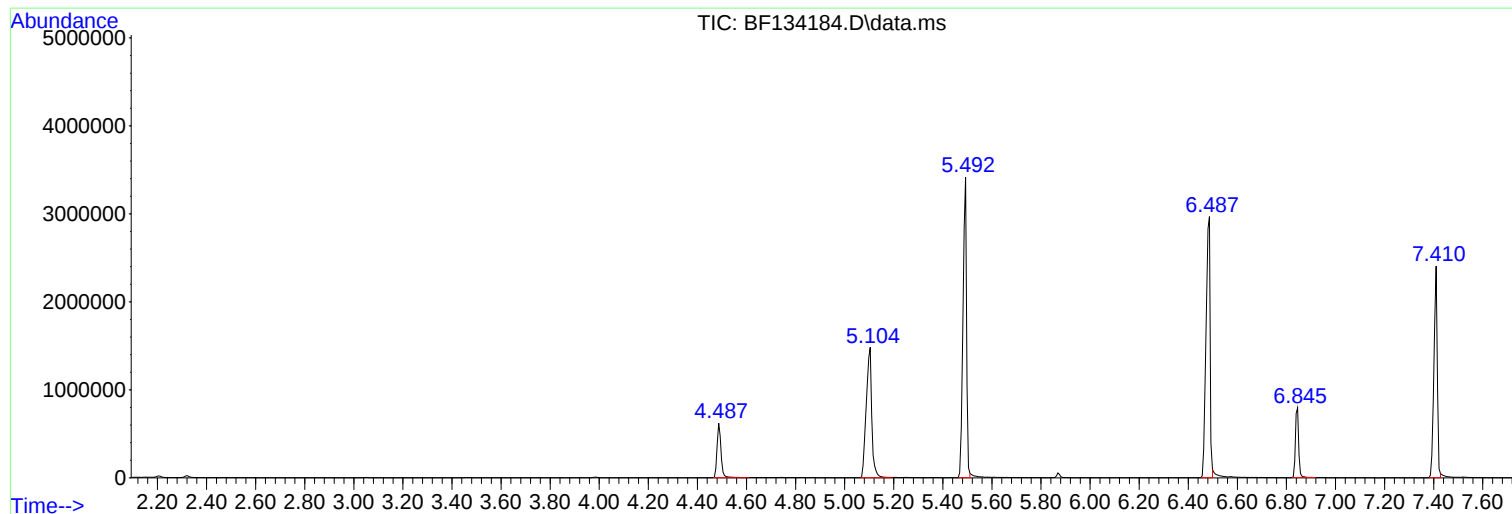
Sum of corrected areas: 30904605

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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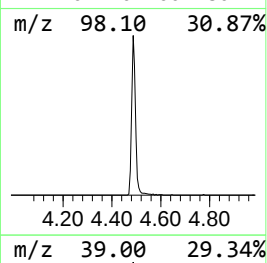
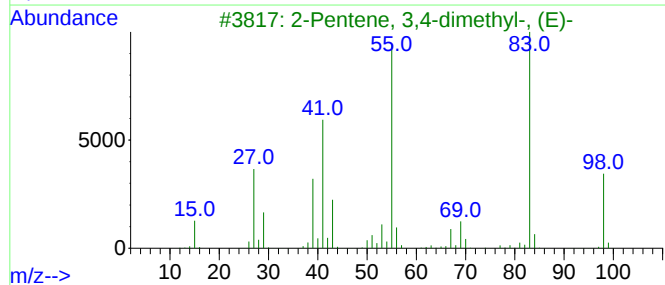
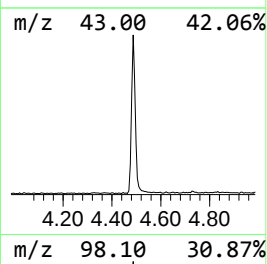
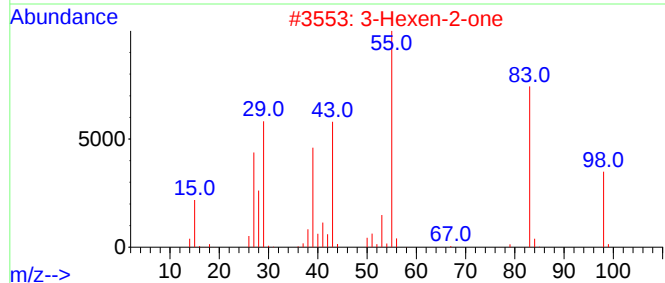
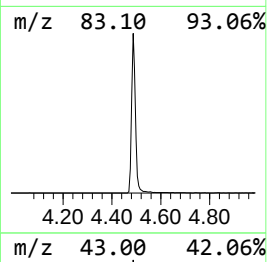
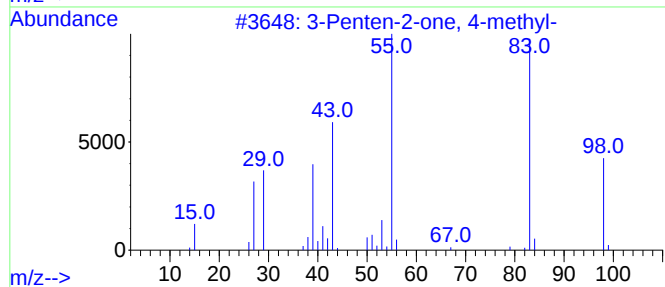
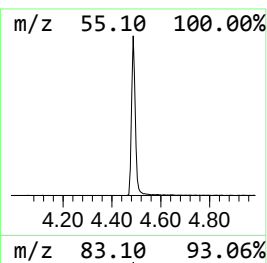
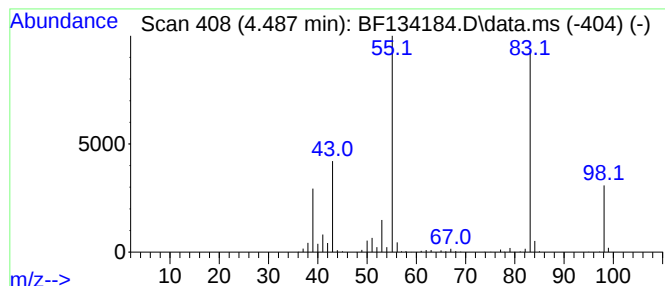
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Peak Number 1 3-Penten-2-one, 4-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.487	19.02 ng	697071	1,4-Dichlorobenzene-d4	6.845

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, 4,4-dimethyl-, (E)-			98	C7H14	000690-08-4	86



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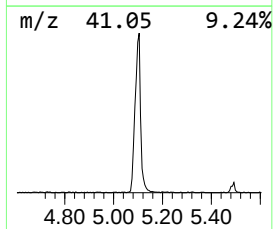
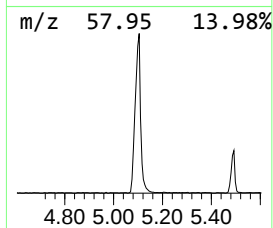
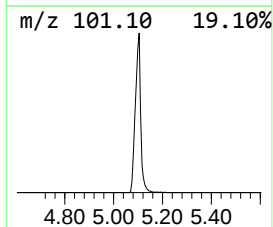
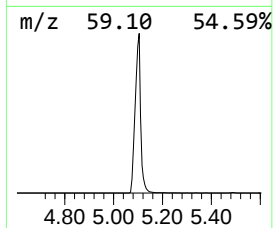
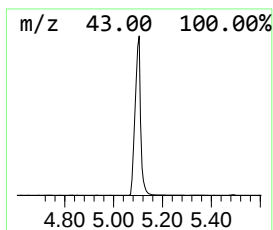
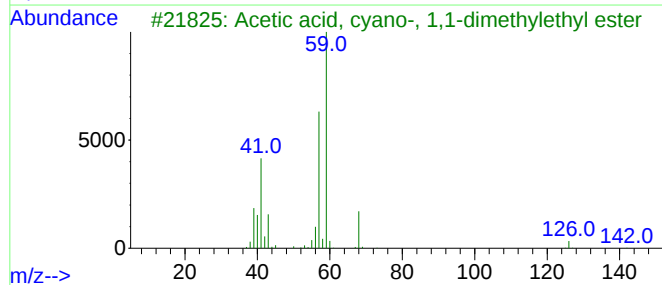
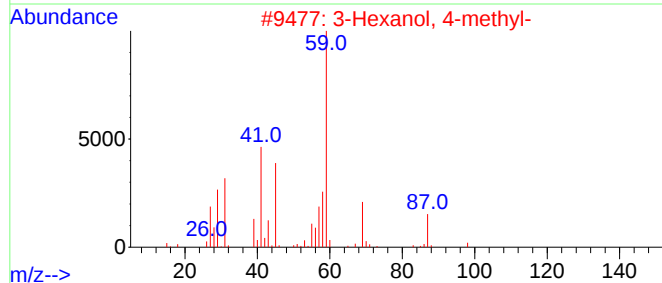
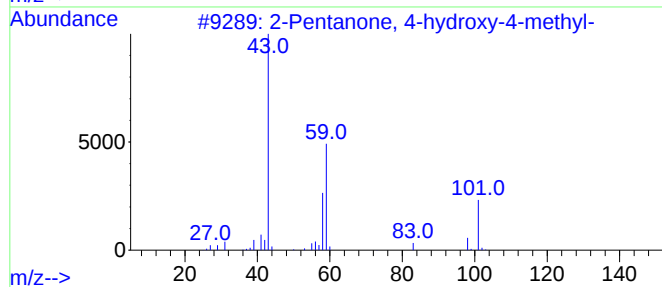
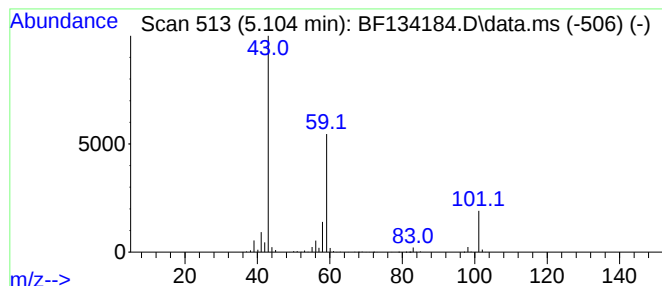
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD			R.T.
5.104	63.04 ng	2310490	1,4-Dichlorobenzene-d4			6.845

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	72
2	3-Hexanol, 4-methyl-	116	C7H16O		000615-29-2	28
3	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2		001116-98-9	17
4	1-Propen-2-ol, acetate	100	C5H8O2		000108-22-5	10
5	Morpholine, 4-methyl-	101	C5H11NO		000109-02-4	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
3-Penten-2-one,...	4.487	19.0	ng	697071	1	6.845	733078	20.0
2-Pentanone, 4-...	5.104	63.0	ng	2310490	1	6.845	733078	20.0