LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130017.D
Acq On : 26 Aug 2022 13:55
Operator : CG\JU
Sample : N4243-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4

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-BF081422.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF130017.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.328	344	347	366	rBV	85155	142587	5.56%	0.795%
2	4.963	452	455	476	rVB	275525	348282	13.59%	1.942%
3	5.387	524	527	551	rBV	1511008	1798432	70.18%	10.029%
4	6.410	698	701	716	rBV	2107354	2011102	78.48%	11.215%
5	6.745	755	758	767	rBV	873314	711624	27.77%	3.969%
6	7.316	852	855	866	rBV	1610730	1371930	53.54%	7.651%
7	8.028	973	976	987	rVB	1160804	961658	37.53%	5.363%
8	9.104	1155	1159	1162	rBV	2998319	2562442	100.00%	14.290%
9	9.780	1271	1274	1278	rBV	1287197	1015717	39.64%	5.664%
10	10.575	1406	1409	1419	rBV	998756	883737	34.49%	4.928%
11	11.269	1524	1527	1530	rBV	1071982	884136	34.50%	4.931%
12	11.292	1530	1531	1536	rVB	130902	109844	4.29%	0.613%
13	11.645	1589	1591	1595	rVB	72699	64422	2.51%	0.359%
14	12.357	1702	1712	1723	rBV2	181717	343889	13.42%	1.918%
15	12.439	1723	1726	1729	rVB	82180	73708	2.88%	0.411%
16	12.486	1731	1734	1739	rBV2	183890	247616	9.66%	1.381%
17	12.716	1768	1773	1779	rVB	138046	156823	6.12%	0.875%
18	12.851	1792	1796	1799	rBV	2132754	1706546	66.60%	9.517%
19	13.286	1866	1870	1872	rBV2	37768	43030	1.68%	0.240%
20	13.327	1872	1877	1883	rVV	662734	604876	23.61%	3.373%
21	13.739	1942	1947	1951	rBV4	21614	32319	1.26%	0.180%
22	13.786	1952	1955	1956	rBV	30482	29913	1.17%	0.167%
23	13.916	1973	1977	1981	rBV	610632	616546	24.06%	3.438%
24	13.945	1981	1982	1985	rVB	62854	43257	1.69%	0.241%
25	14.004	1988	1992	1995	rBV	111401	110497	4.31%	0.616%
26	14.651	2099	2102	2105	rVB4	26233	29437	1.15%	0.164%
27	14.798	2123	2127	2131	rBV3	43774	52119	2.03%	0.291%
28	14.951	2150	2153	2155	rBV	83277	102563	4.00%	0.572%
29	15.245	2200	2203	2209	rVB	47588	56298	2.20%	0.314%
30	15.310	2211	2214	2219	rBV	65150	81522	3.18%	0.455%
31	15.362	2219	2223	2229	rBV	479875	568003	22.17%	3.168%
32	15.527	2247	2251	2256	rBV4	36371	54672	2.13%	0.305%
33	15.739	2284	2287	2292	rVB2	38200	53022	2.07%	0.296%
34	16.821	2468	2471	2478	rVB2	29971	58934	2.30%	0.329%

Sum of corrected areas: 17931503

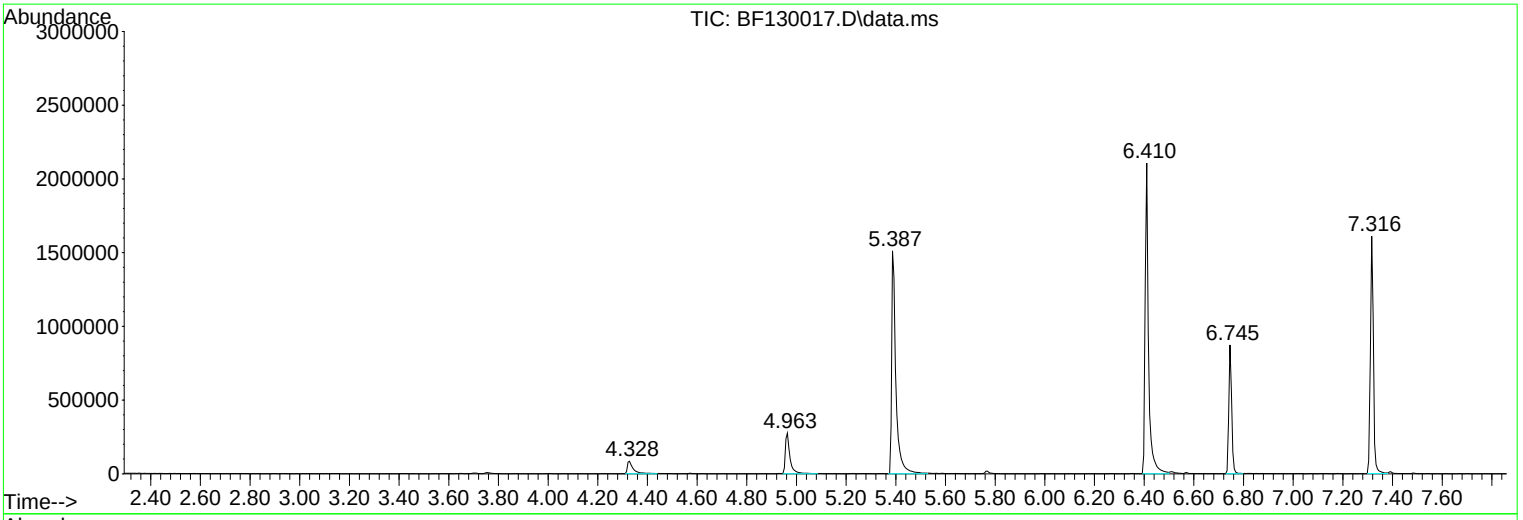
Instrument :
BNA_F
ClientSampleId :
B-4

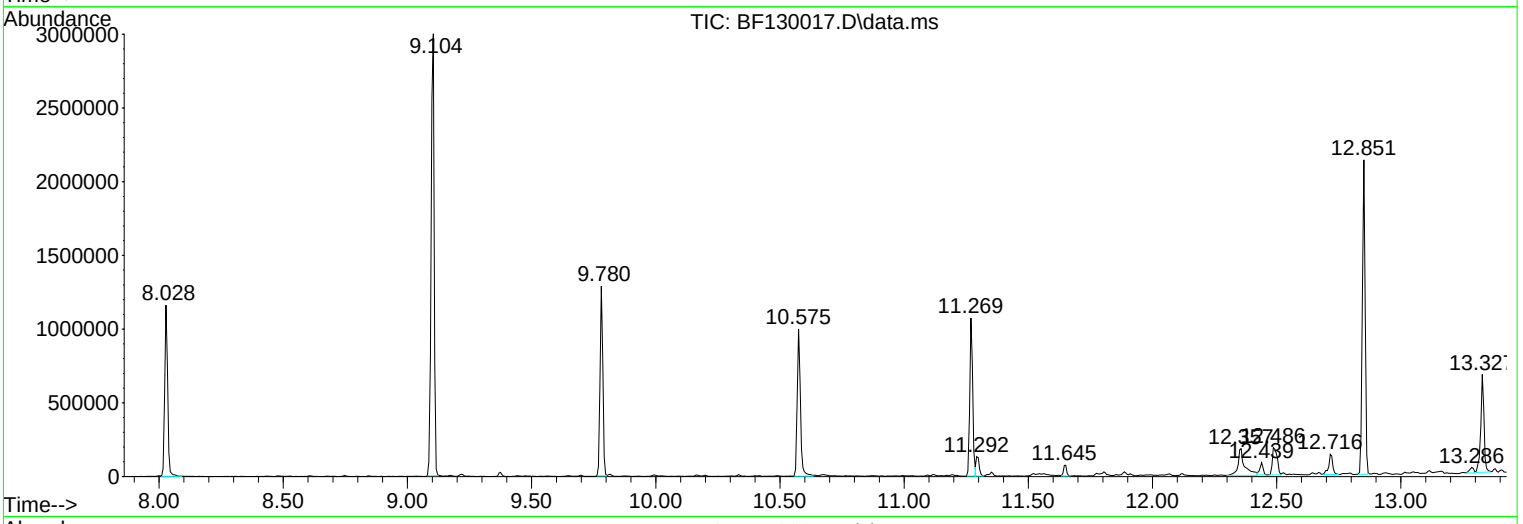
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF082622\
Data File : BF130017.D
Acq On : 26 Aug 2022 13:55
Operator : CG\JU
Sample : N4243-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

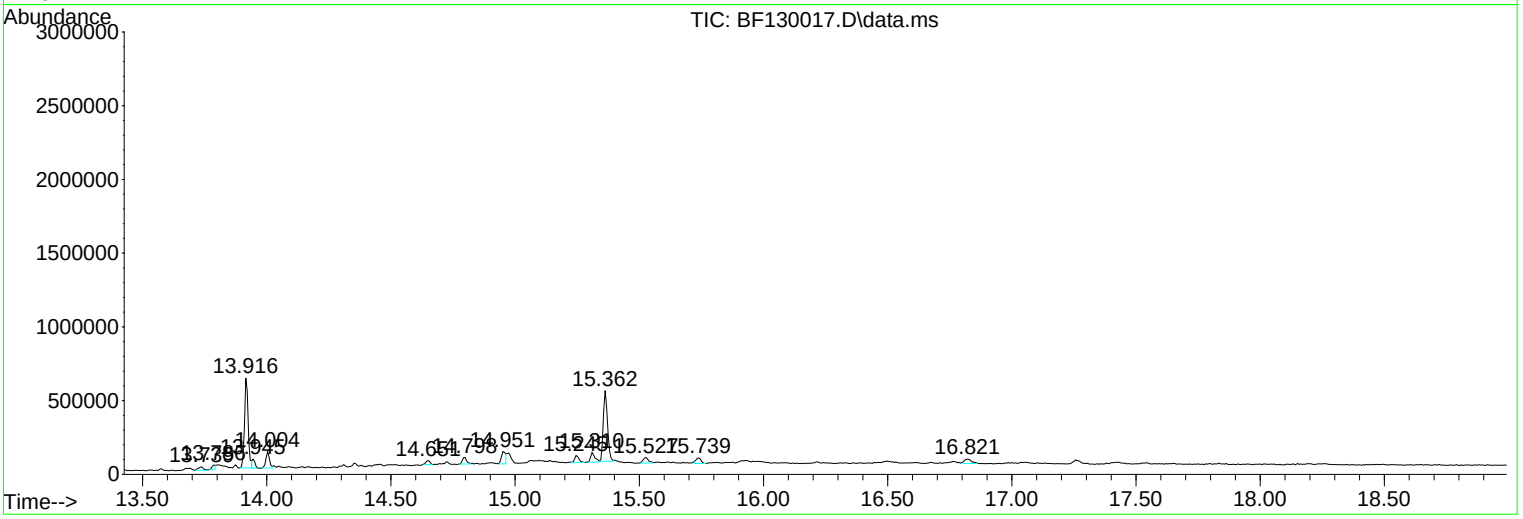
Instrument :
BNA_F
ClientSampleId :
B-4

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.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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Data File : BF130017.D
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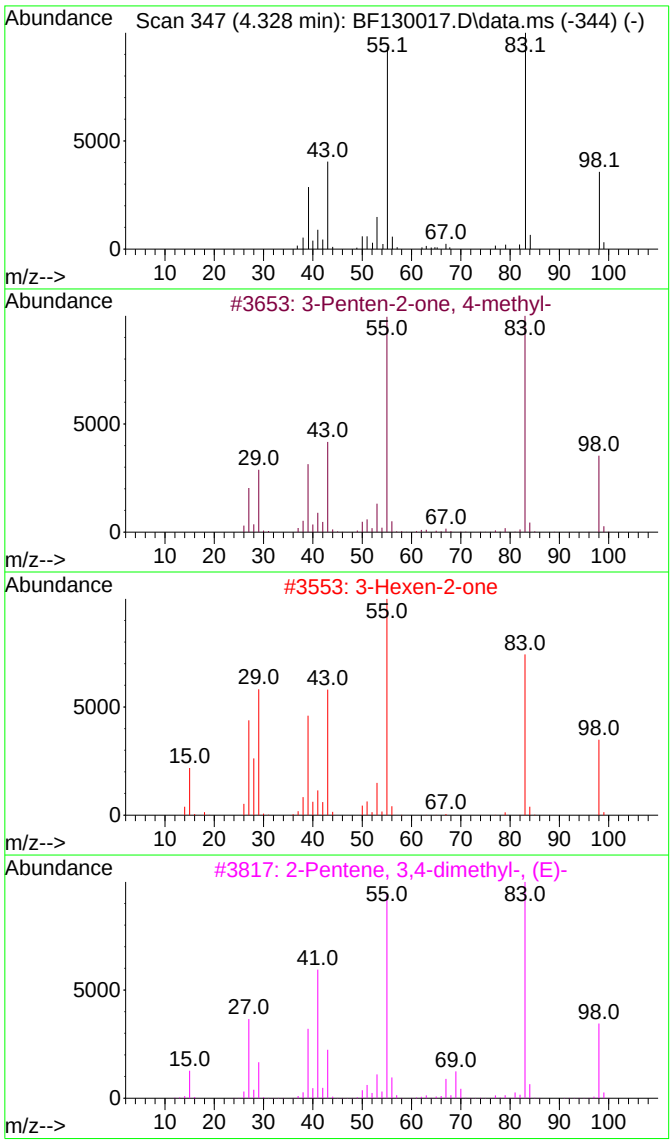
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

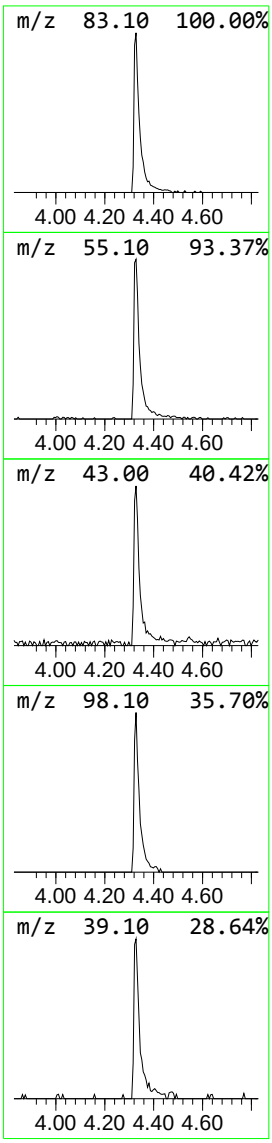
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.328	4.01 ng	142587	1,4-Dichlorobenzene-d4	6.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	95
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, 2,4-dimethyl-	98	C7H14	000625-65-0	87
5	2-Pentene, 4,4-dimethyl-, (E)-	98	C7H14	000690-08-4	86





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Data File : BF130017.D
Acq On : 26 Aug 2022 13:55
Operator : CG\JU
Sample : N4243-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
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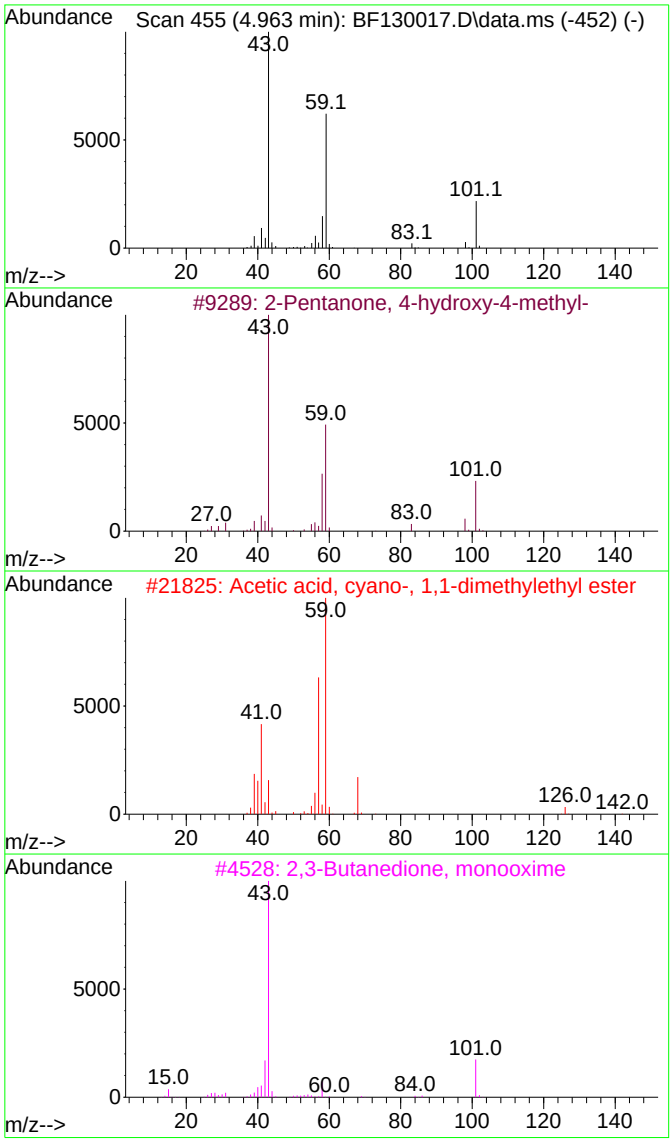
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

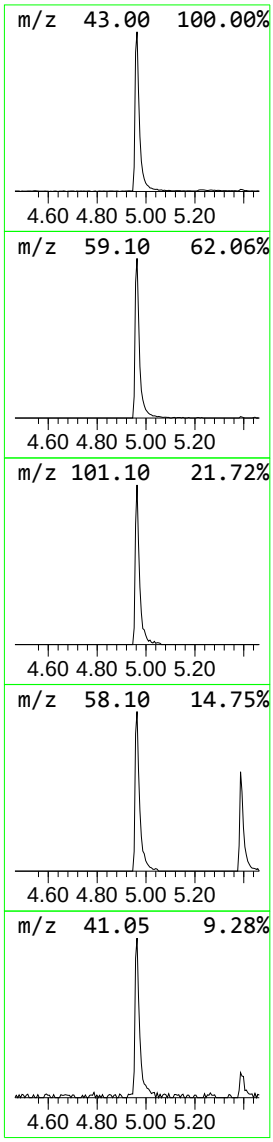
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.963	9.79 ng	348282	1,4-Dichlorobenzene-d4	6.745

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	40
2	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	32
3	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
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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Data File : BF130017.D
Acq On : 26 Aug 2022 13:55
Operator : CG\JU
Sample : N4243-01
Misc :
ALS Vial : 6 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
B-4

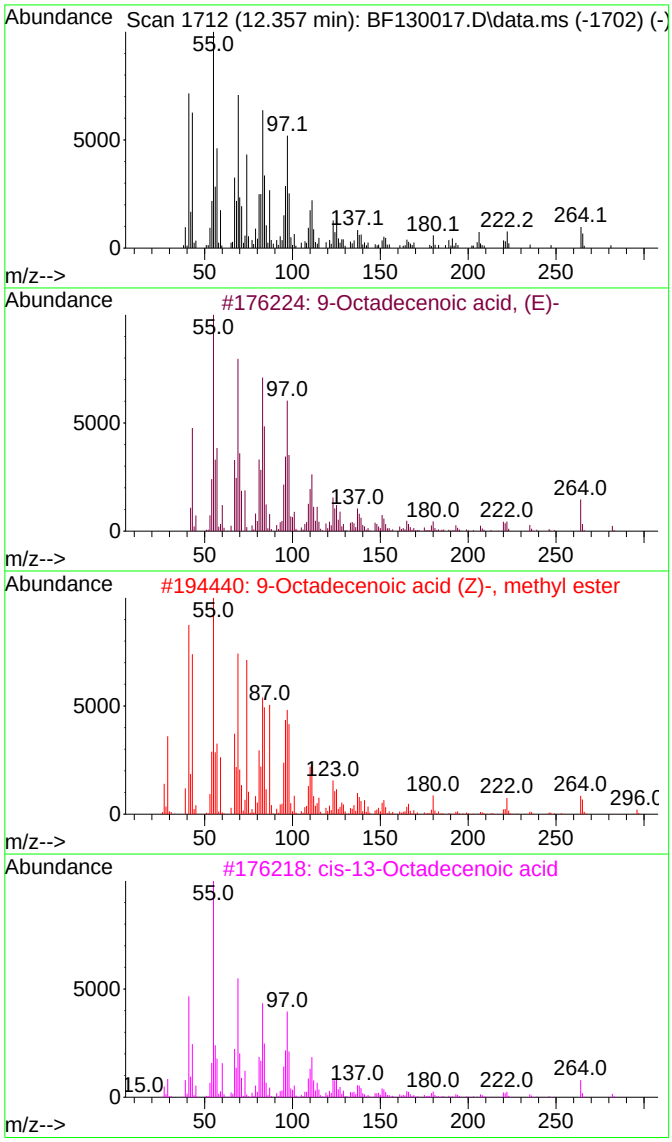
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

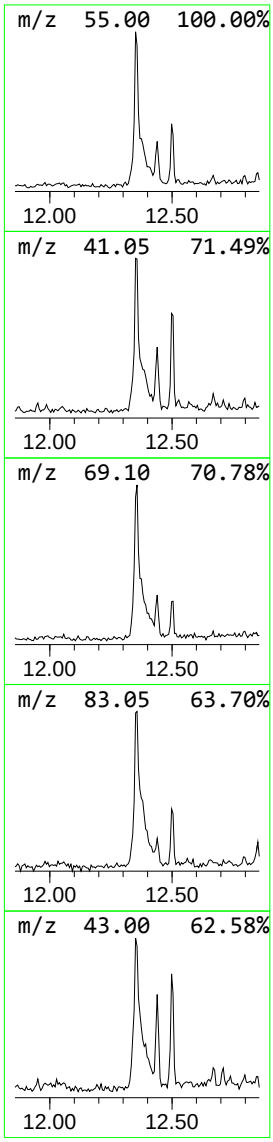
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 9-Octadecenoic acid, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.357	7.78 ng	343889	Phenanthrene-d10	11.269

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenoic acid, (E)-	282	C18H34O2	000112-79-8	86
2	9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	76
3	cis-13-Octadecenoic acid	282	C18H34O2	013126-39-1	70
4	cis-Vaccenic acid	282	C18H34O2	000506-17-2	70
5	Oleic Acid	282	C18H34O2	000112-80-1	62





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Instrument :
BNA_F
ClientSampleId :
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

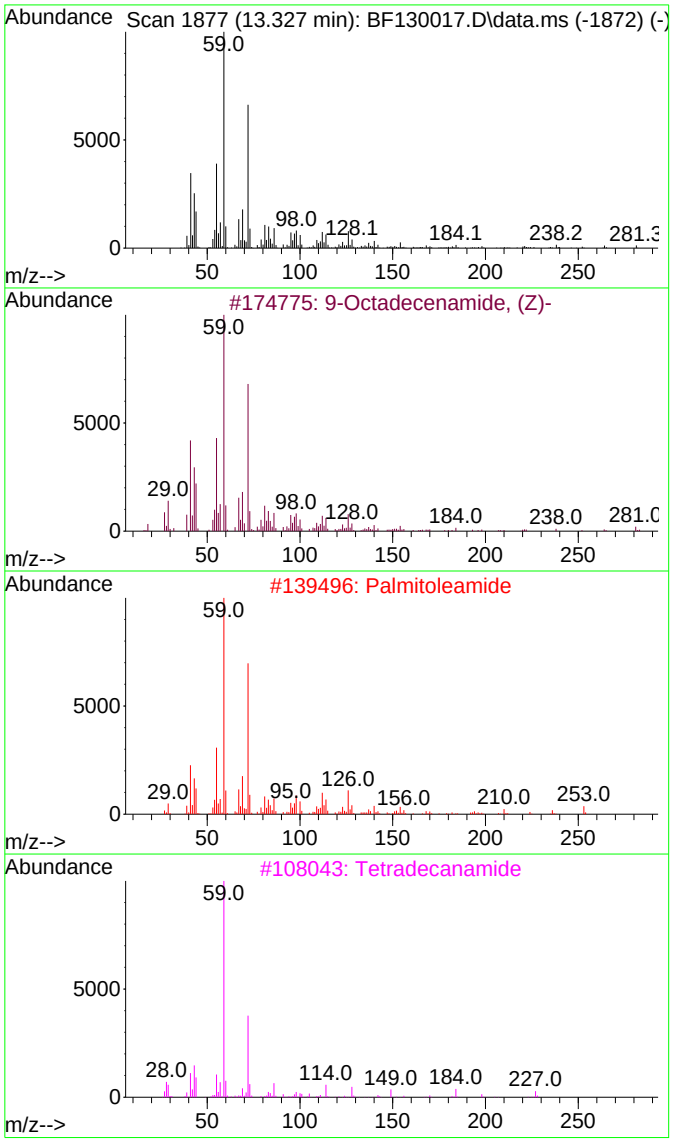
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

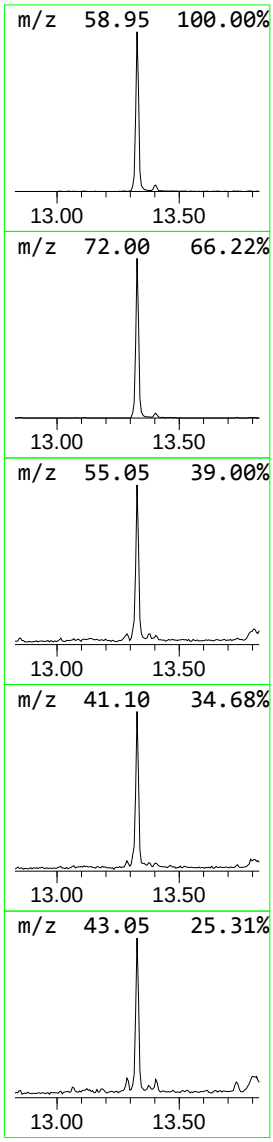
****

Peak Number 4 9-Octadecenamide, (Z)- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.327	19.62 ng	604876	Chrysene-d12	13.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	98
2	Palmitoleamide	253	C16H31NO	106010-22-4	91
3	Tetradecanamide	227	C14H29NO	000638-58-4	64
4	Dodecanamide	199	C12H25NO	001120-16-7	64
5	Nonanamide	157	C9H19NO	001120-07-6	64





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Instrument :
BNA_F
ClientSampleId :
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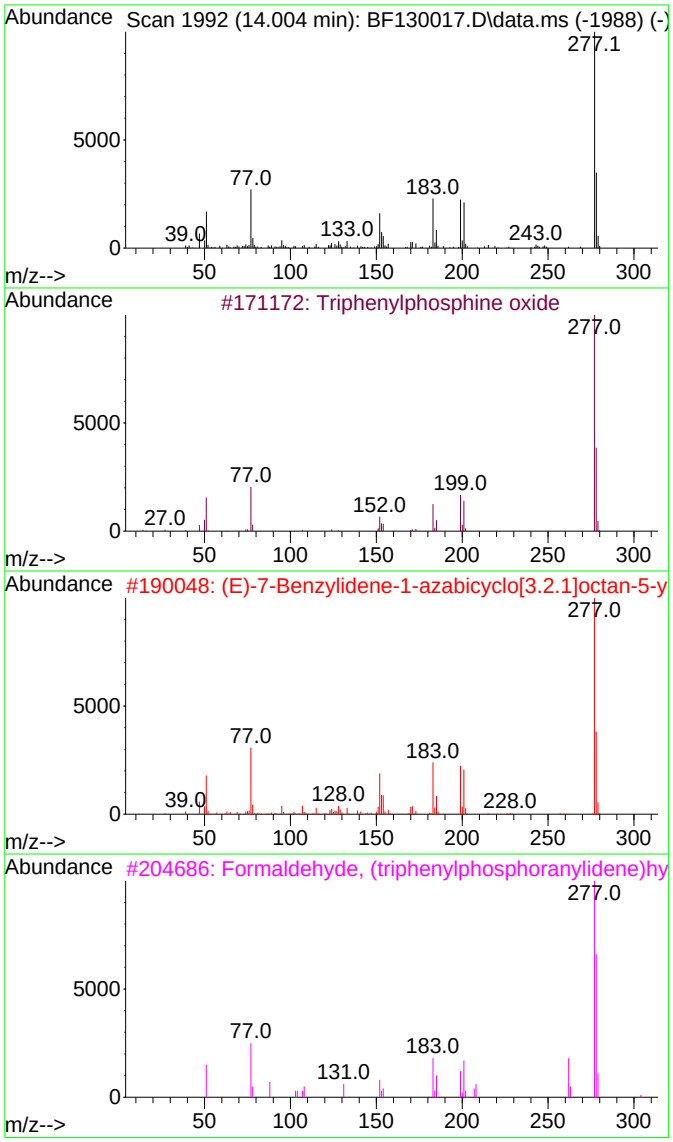
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

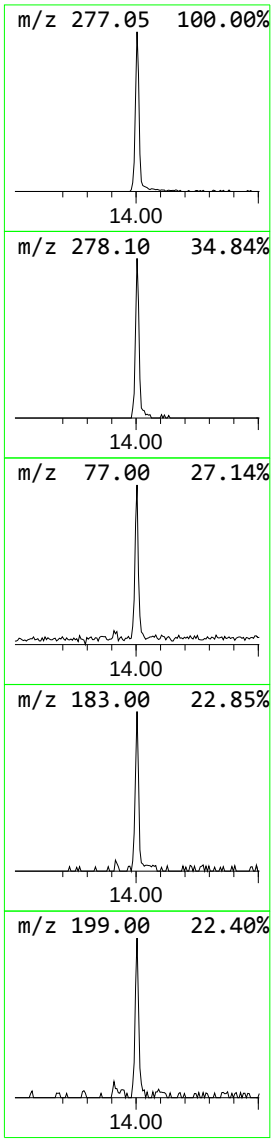
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 Triphenylphosphine oxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.004	3.58 ng	110497	Chrysene-d12	13.916

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Triphenylphosphine oxide	278	C18H15OP	000791-28-6	94
2	(E)-7-Benzylidene-1-azabicyclo[3...	293	C15H19NO3S	1000483-83-4	91
3	Formaldehyde, (triphenylphosphor...	304	C19H17N2P	015990-54-2	50
4	4-Nitro-4'-methyldiphenylsulfone	277	C13H11NO4S	004094-37-5	43
5	Cyclotrisiloxane, hexaethyl-	306	C12H30O3Si3	002031-79-0	27





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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF081422.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

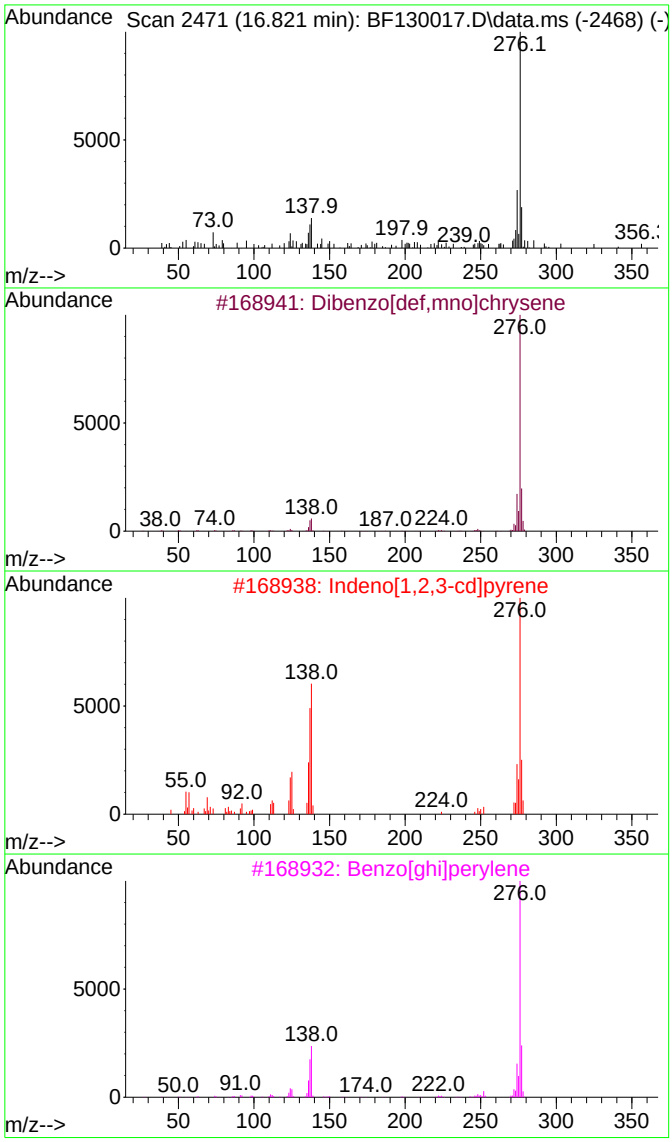
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

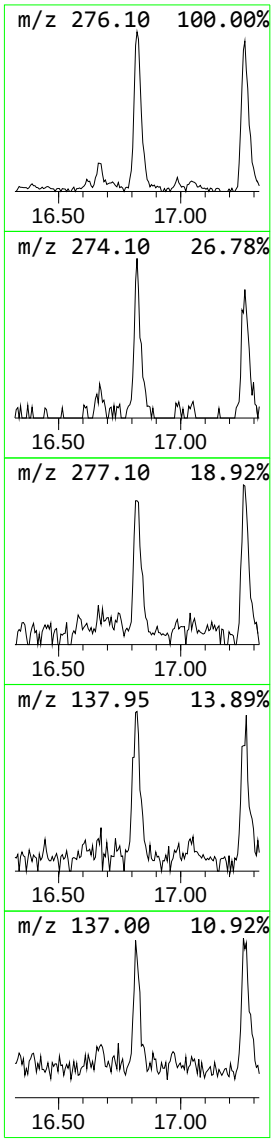
****

Peak Number 6 Dibenzo[def,mno]chrysene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.821	2.08 ng	58934	Perylene-d12	15.363

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dibenzo[def,mno]chrysene	276	C22H12	000191-26-4	58
2	Indeno[1,2,3-cd]pyrene	276	C22H12	000193-39-5	58
3	Benzo[ghi]perylene	276	C22H12	000191-24-2	53
4	12H-Benzothieno[2,3-d]pyrido[1,2...	276	C14H16N2S2	102254-63-7	53
5	2-(p-Tolyl)oxazolo[4,5-c]quinoli...	276	C17H12N2O2	148563-22-8	50





Tentatively Identified Compound (LSC) summary

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Instrument :
BNA_F
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
3-Penten-2-one,...	4.328	4.0	ng	142587	1	6.745	711624	20.0
2-Pentanone, 4-...	4.963	9.8	ng	348282	1	6.745	711624	20.0
9-Octadecenoic ...	12.357	7.8	ng	343889	4	11.269	884136	20.0
9-Octadecenamid...	13.327	19.6	ng	604876	5	13.916	616546	20.0
Triphenylphosph...	14.004	3.6	ng	110497	5	13.916	616546	20.0
Dibenzo[def,mno...	16.821	2.1	ng	58934	6	15.363	568003	20.0