LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013244.D
Acq On : 22 Dec 2022 13:57
Operator : CG/JU
Sample : N6015-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument : BNA_P
ClientSampleId : DBXT7

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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\SFAM-EPA-BP120722.M
Title : SVOA CALIBRATION

Signal : TIC: BP013244.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.334	21	25	34	rVB	238361	305068	0.44%	0.104%
2	3.758	94	97	113	rBV	2307593	3534492	5.06%	1.210%
3	4.093	150	154	160	rVB	53867	75045	0.11%	0.026%
4	7.110	658	667	679	rBV	3850205	6200048	8.88%	2.123%
5	7.275	686	695	705	rBV	3130578	4807535	6.88%	1.646%
6	7.475	722	729	740	rBV	3941863	6168991	8.83%	2.112%
7	7.946	802	809	816	rBV	2607166	4035001	5.78%	1.381%
8	8.657	919	930	940	rBV	4763223	7631245	10.92%	2.613%
9	9.116	1000	1008	1016	rBV	3855924	6154192	8.81%	2.107%
10	9.516	1070	1076	1083	rVB	57495	92106	0.13%	0.032%
11	9.704	1101	1108	1114	rVB	191866	298316	0.43%	0.102%
12	9.840	1122	1131	1147	rBV	3287422	5402475	7.73%	1.850%
13	10.381	1215	1223	1241	rBV	4976329	8395016	12.02%	2.874%
14	10.763	1278	1288	1299	rBV	3567676	6090432	8.72%	2.085%
15	10.898	1303	1311	1333	rVV	3818143	6602488	9.45%	2.261%
16	11.140	1343	1352	1361	rVV2	95656	178321	0.26%	0.061%
17	11.228	1361	1367	1375	rVB2	66441	109263	0.16%	0.037%
18	12.340	1551	1556	1561	rBV	82939	125014	0.18%	0.043%
19	13.404	1727	1737	1743	rBV2	74038	122783	0.18%	0.042%
20	13.510	1750	1755	1760	rBV2	45966	73235	0.10%	0.025%
21	13.575	1760	1766	1772	rVB	393752	564740	0.81%	0.193%
22	13.998	1830	1838	1847	rBV	8385986	11454337	16.40%	3.922%
23	14.286	1879	1887	1905	rVB	9617017	14348554	20.54%	4.913%
24	14.475	1910	1919	1926	rVB3	43218	92478	0.13%	0.032%
25	14.586	1928	1938	1947	rBV	5447468	8264948	11.83%	2.830%
26	14.786	1965	1972	1990	rBV	3067410	4708575	6.74%	1.612%
27	14.939	1995	1998	2003	rVV4	45335	76343	0.11%	0.026%
28	14.992	2003	2007	2014	rVB9	43763	74951	0.11%	0.026%
29	15.581	2100	2107	2120	rBV	11666152	17467856	25.00%	5.981%
30	15.704	2121	2128	2138	rVV	3725771	5085073	7.28%	1.741%
31	15.822	2144	2148	2158	rVB	61894	106324	0.15%	0.036%
32	15.945	2160	2169	2176	rBV	2078917	2824414	4.04%	0.967%
33	17.210	2379	2384	2385	rBV2	69879	97601	0.14%	0.033%
34	17.345	2401	2407	2417	rBV	6501112	9575489	13.71%	3.278%
35	17.445	2417	2424	2432	rVV	12217139	17035576	24.39%	5.833%
36	17.698	2464	2467	2470	rBV3	73910	95793	0.14%	0.033%

LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013244.D
Acq On : 22 Dec 2022 13:57
Operator : CG/JU
Sample : N6015-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXT7

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 0.1 % 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\SFAM-EPA-BP120722.M
Title : SVOA CALIBRATION

37	18.151	2540	2544	2549	rBV3	150871	209338	0.30%	0.072%
38	18.216	2550	2555	2566	rBV	1369727	2045652	2.93%	0.700%
39	18.551	2608	2612	2618	rVV5	55131	91516	0.13%	0.031%
40	19.251	2728	2731	2737	rVB	151056	209276	0.30%	0.072%
41	19.322	2737	2743	2746	rBV2	255051	542748	0.78%	0.186%
42	19.445	2761	2764	2778	rBV	287102	407272	0.58%	0.139%
43	19.680	2798	2804	2814	rVB	12975208	17400699	24.91%	5.958%
44	20.880	2990	3008	3028	rVB2	14499728	69859283	100.00%	23.918%
45	21.127	3045	3050	3052	rBV	2278678	3377397	4.83%	1.156%
46	21.433	3097	3102	3106	rBV	5572917	7906524	11.32%	2.707%
47	23.751	3489	3496	3509	rVB2	7572010	15203792	21.76%	5.205%
48	23.910	3516	3523	3537	rVB2	3514227	7407024	10.60%	2.536%
49	24.521	3624	3627	3637	rVB	785369	1551466	2.22%	0.531%
50	28.986	4378	4386	4400	rVB3	2081861	7592757	10.87%	2.600%

Sum of corrected areas: 292078862

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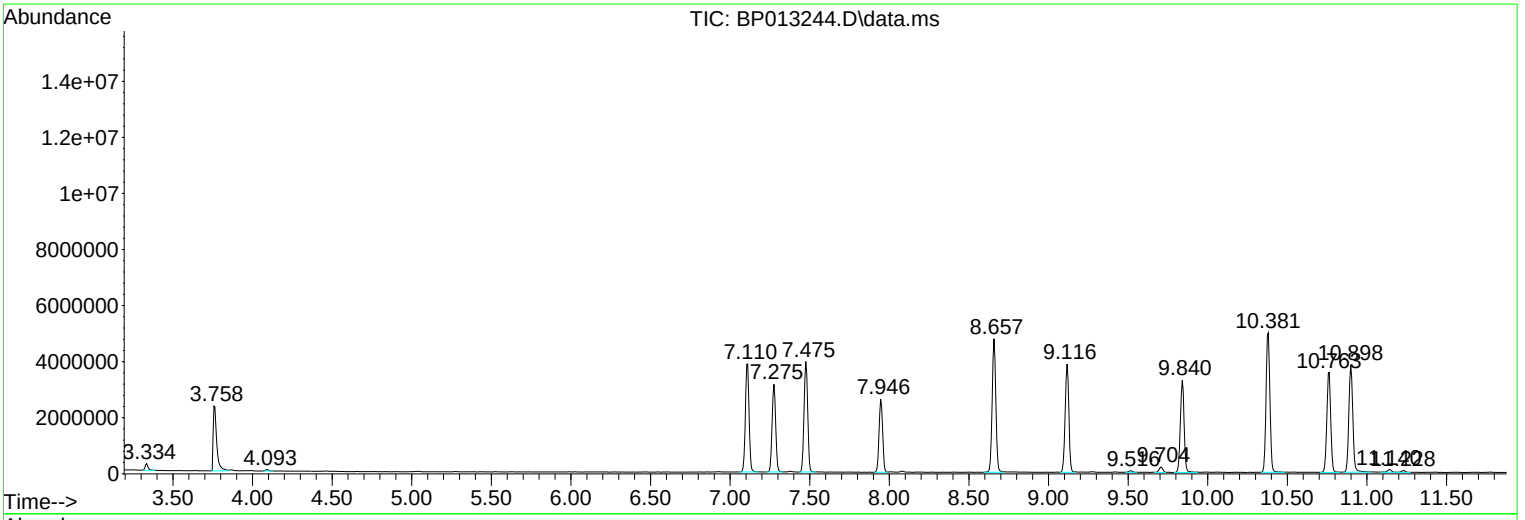
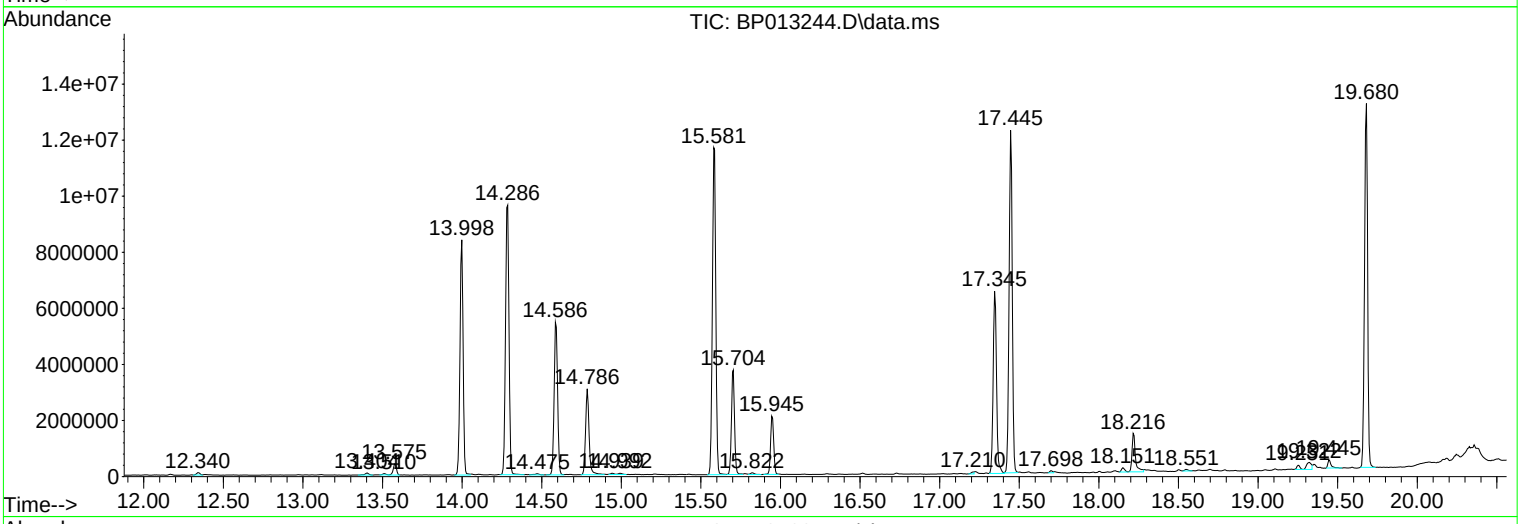
ALS Vial : 11 Sample Multiplier: 1

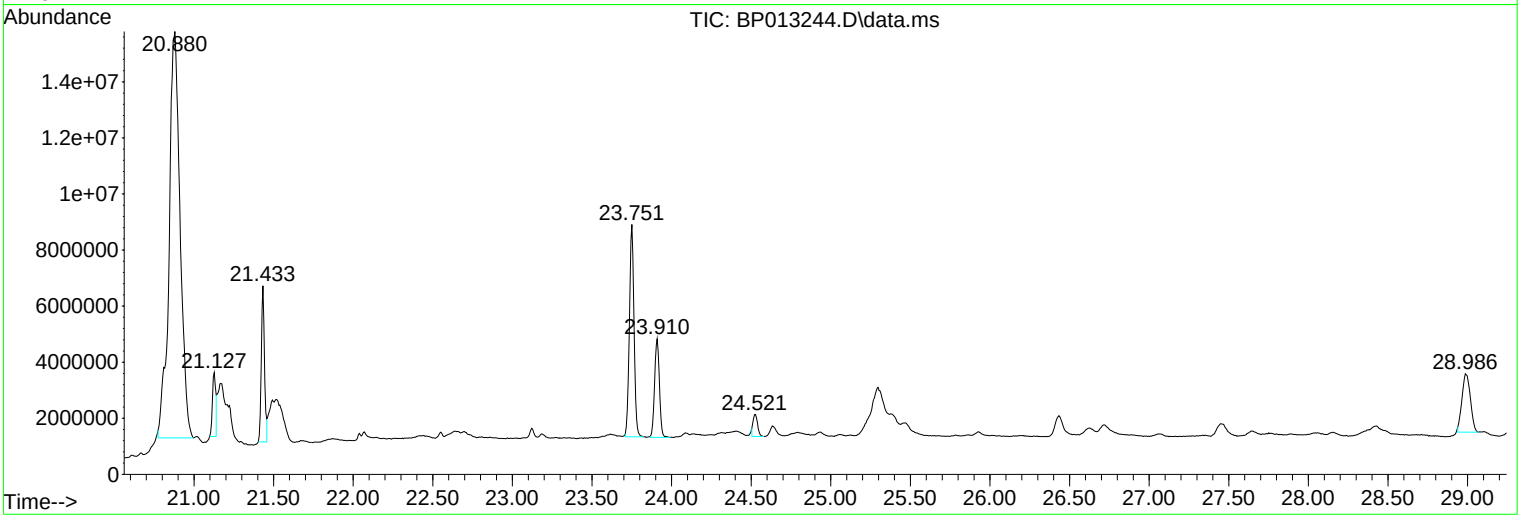
Instrument :
BNA_P
ClientSampleId :
DBXT7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

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







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Data File : BP013244.D
Acq On : 22 Dec 2022 13:57
Operator : CG/JU
Sample : N6015-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

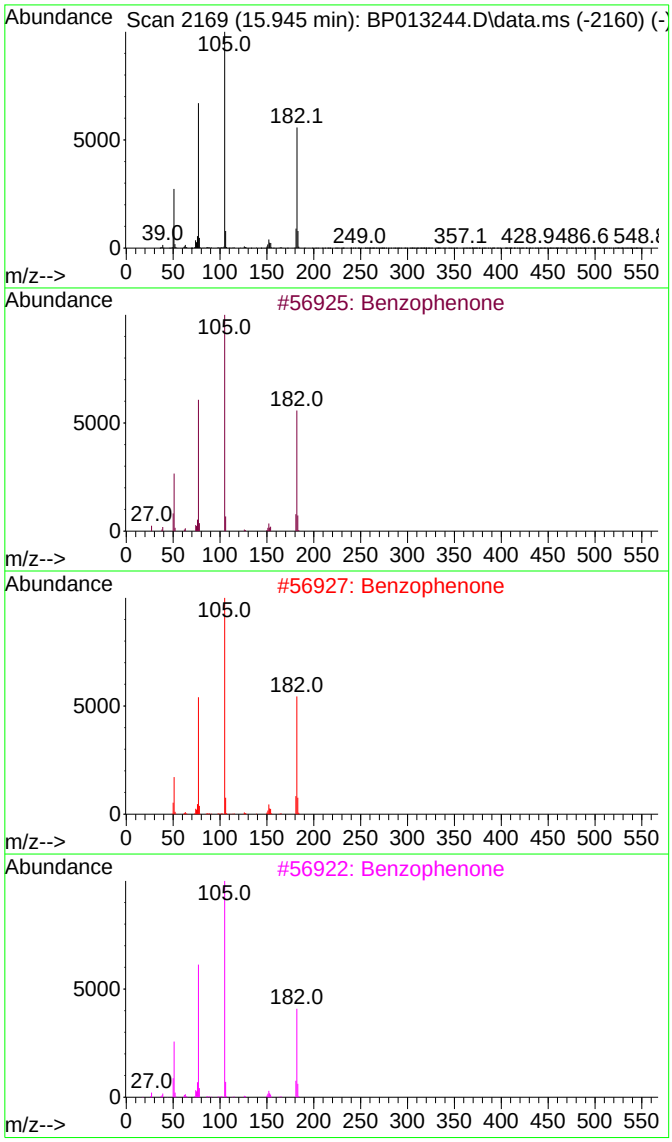
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

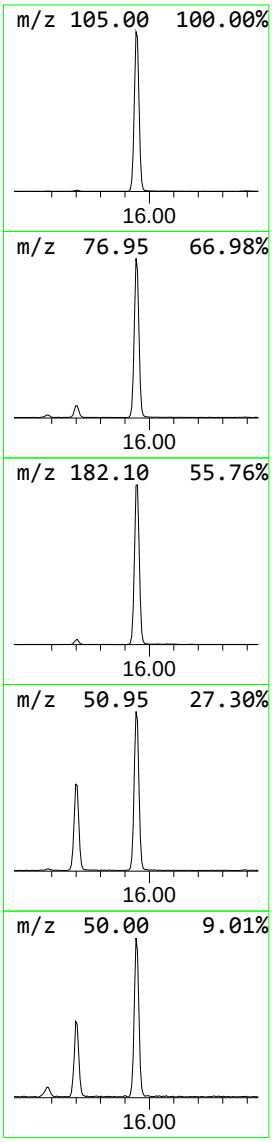
****

Peak Number 1 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.945	6.83 ng/ul	2824410	Acenaphthene-d10	14.586

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Benzophenone	182	C13H10O	000119-61-9	95
3	Benzophenone	182	C13H10O	000119-61-9	94
4	Benzophenone	182	C13H10O	000119-61-9	91
5	Benzophenone	182	C13H10O	000119-61-9	90





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013244.D
Acq On : 22 Dec 2022 13:57
Operator : CG/JU
Sample : N6015-03
Misc :
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Instrument :
BNA_P
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

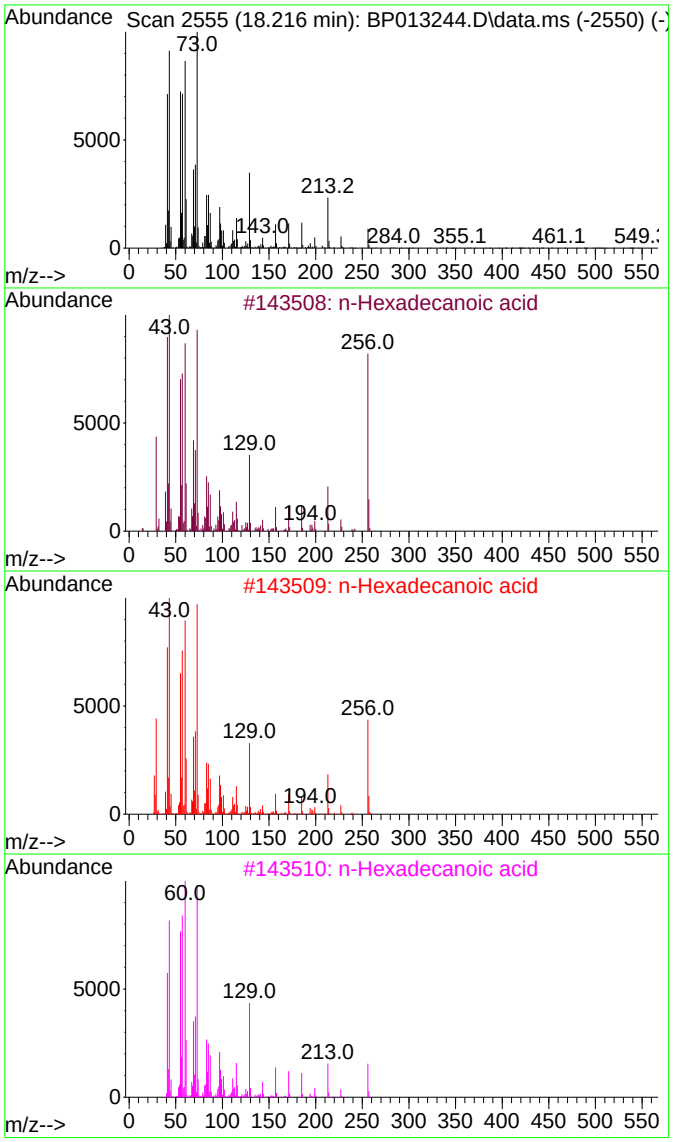
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

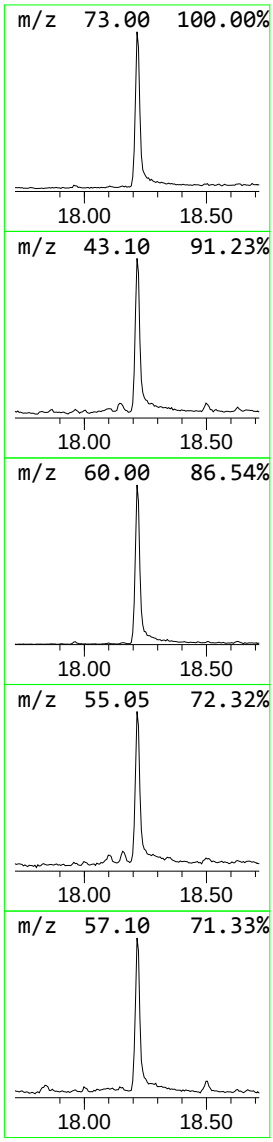
****

Peak Number 2 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.216	4.27 ng/ul	2045650	Phenanthrene-d10	17.345

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
4	Tridecanoic acid	214	C13H26O2	000638-53-9	95
5	Tetradecanoic acid	228	C14H28O2	000544-63-8	93





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013244.D
Acq On : 22 Dec 2022 13:57
Operator : CG/JU
Sample : N6015-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXT7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

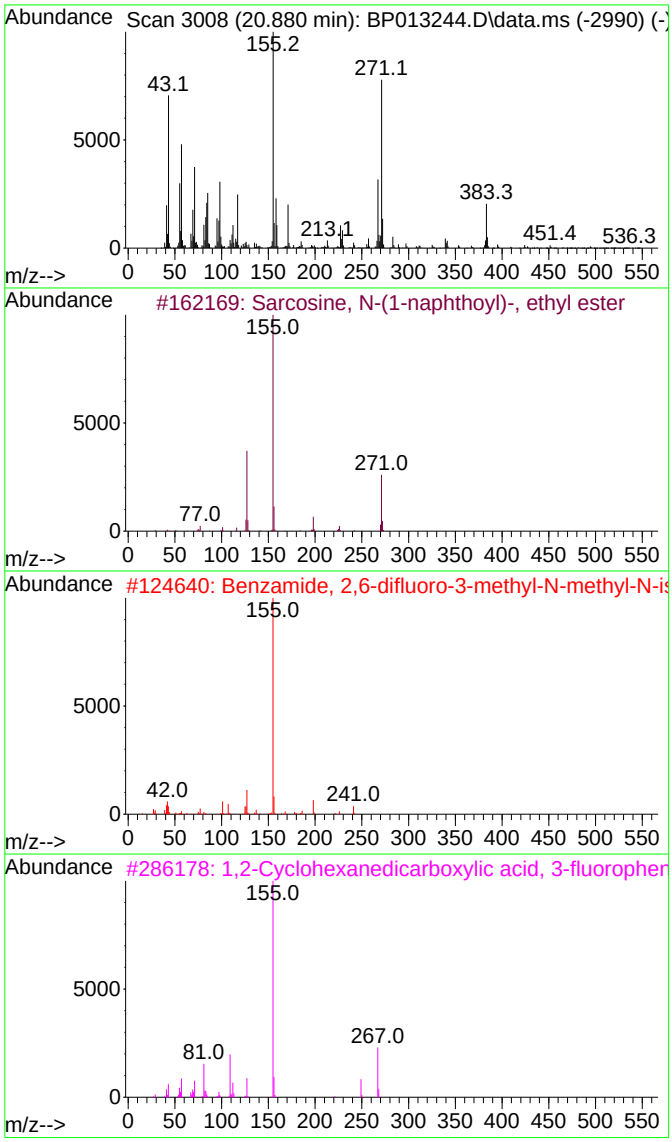
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

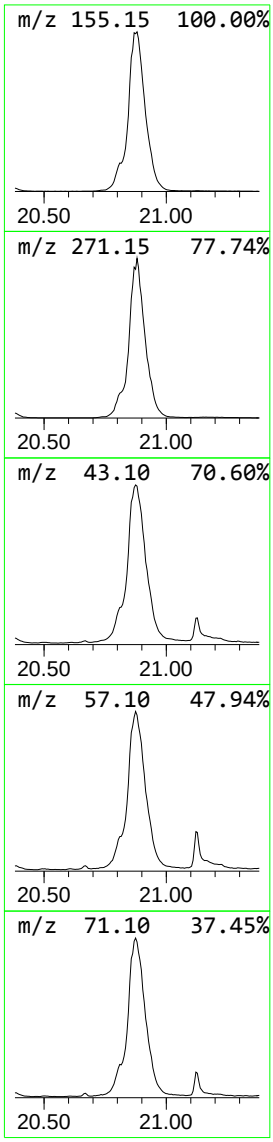
****

Peak Number 3 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.880	176.71 ng/ul	69859300	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Sarcosine, N-(1-naphthoyl)-, eth...	271	C16H17NO3	1000321-39-8	35
2	Benzamide, 2,6-difluoro-3-methyl...	241	C13H17F2NO	1000437-11-2	35
3	1,2-Cyclohexanedicarboxylic acid...	378	C22H31FO4	1000339-40-2	22
4	7H-[1,3,4]Thiadiazolo[3,2-a]pyri...	271	C9H9N3O3S2	1000350-95-4	20
5	(+)-4-Methoxy-6-ketomorphinan	271	C17H21NO2	1000129-08-5	18





Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013244.D
Acq On : 22 Dec 2022 13:57
Operator : CG/JU
Sample : N6015-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXT7

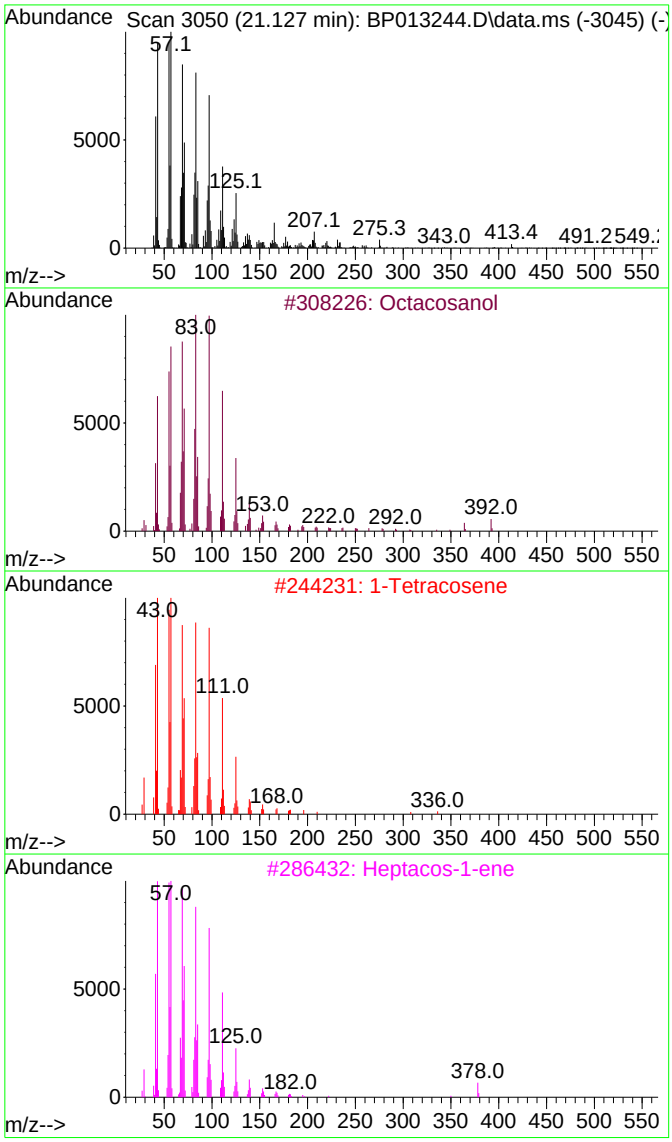
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

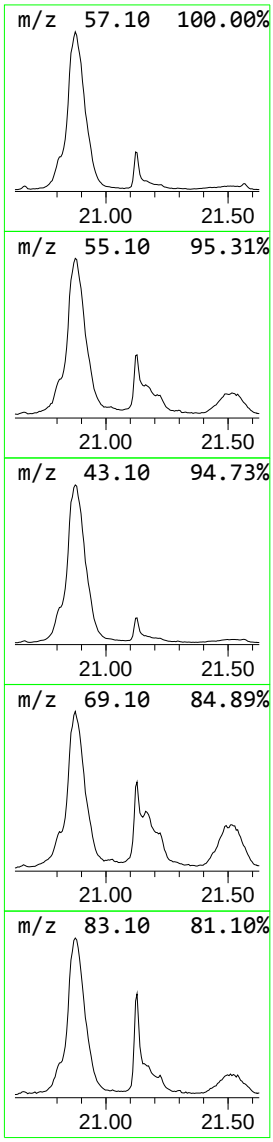
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 4 Octacosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.127	8.54 ng/ul	3377400	Chrysene-d12	21.433

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octacosanol	410	C28H58O	000557-61-9	90
2	1-Tetracosene	336	C24H48	010192-32-2	90
3	Heptacos-1-ene	378	C27H54	015306-27-1	90
4	Nonacos-1-ene	406	C29H58	018835-35-3	90
5	1-Heptacosanol	396	C27H56O	002004-39-9	90





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Data File : BP013244.D
Acq On : 22 Dec 2022 13:57
Operator : CG/JU
Sample : N6015-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
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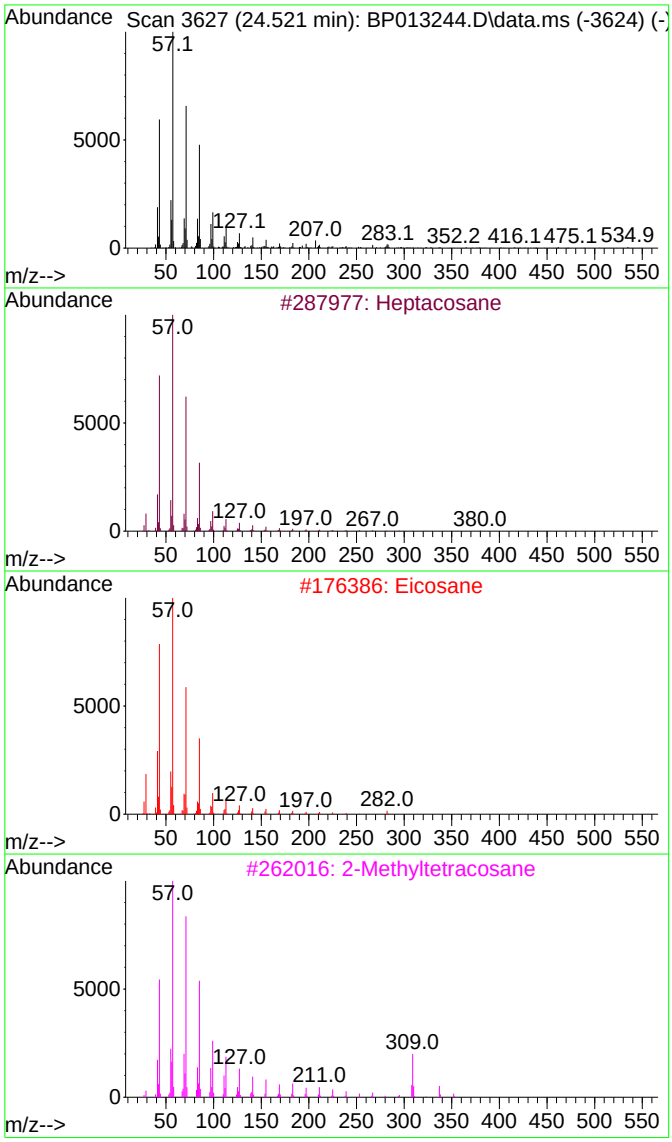
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

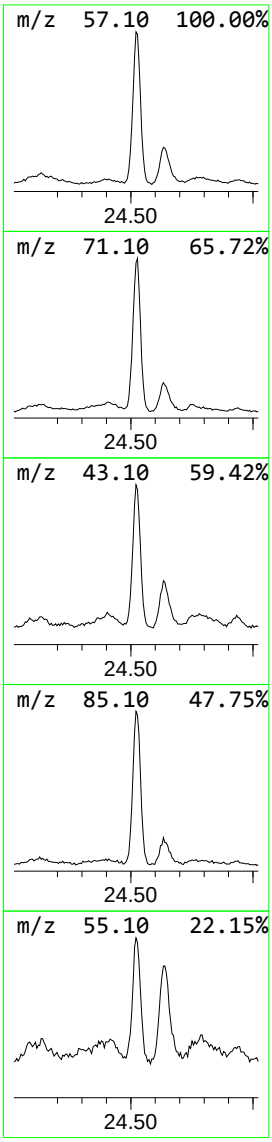
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 5 (DEL) Alkane: Straight-Chai... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.521	4.19 ng/ul	1551470	Perylene-d12	23.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptacosane	380	C27H56	000593-49-7	94
2	Eicosane	282	C20H42	000112-95-8	93
3	2-Methyltetracosane	352	C25H52	001560-78-7	93
4	Heptadecane	240	C17H36	000629-78-7	91
5	Eicosane	282	C20H42	000112-95-8	91





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Data File : BP013244.D
Acq On : 22 Dec 2022 13:57
Operator : CG/JU
Sample : N6015-03
Misc :
ALS Vial : 11 Sample Multiplier: 1

Instrument :
BNA_P
ClientSampleId :
DBXT7

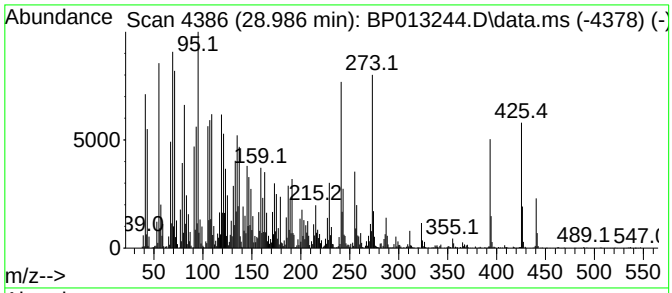
Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA CALIBRATION

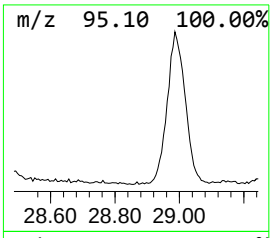
TIC Library : C:\DATABASE\NIST20.L
TIC Integration Parameters: LSCINT.P

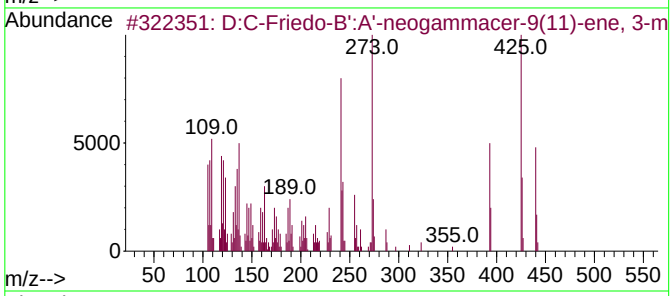
****
Peak Number 6 D:C-Friedo-B':A'-neogammace... Concentration Rank 2

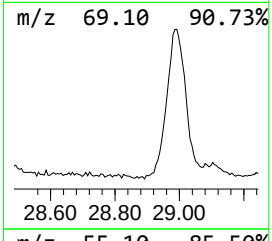
R.T.	EstConc	Area	Relative to ISTD	R.T.
28.986	20.50 ng/ul	7592760	Perylene-d12	23.910

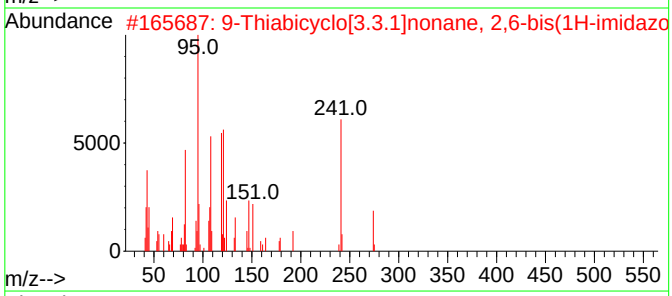
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	D:C-Friedo-B':A'-neogammacer-9(1...	440	C31H52O	004555-56-0	78
2	9-Thiabicyclo[3.3.1]nonane, 2,6-...	274	C14H18N4S	1000141-52-1	30
3	Androst-5-ene-3,19-diol, 3-aceta...	332	C21H32O3	055320-48-4	25
4	5-(3-Hydroxy-4,4,10,13,14-pentam...	558	C34H54O6	1000495-09-3	22
5	Lupeol	426	C30H50O	000545-47-1	20

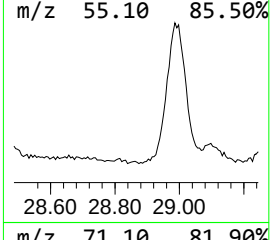


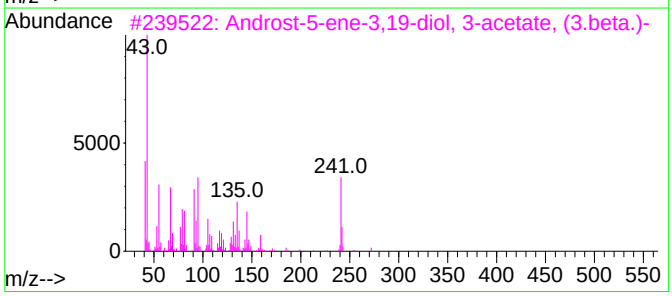


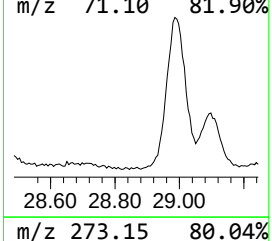


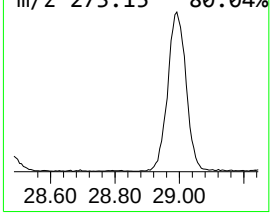












Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_P\Data\BP122222\
Data File : BP013244.D
Acq On : 22 Dec 2022 13:57
Operator : CG/JU
Sample : N6015-03
Misc :
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ClientSampleId :
DBXT7

Quant Method : Z:\svoasrv\HPCHEM1\BNA_P\Methods\SFAM-EPA-BP120722.M
Quant Title : SVOA 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
Benzophenone	15.945	6.8	ng/ul	2824410	3	14.586	8264950	20.0
n-Hexadecanoic ...	18.216	4.3	ng/ul	2045650	4	17.345	9575490	20.0
unknown-01	20.880	176.7	ng/ul	69859300	5	21.433	7906520	20.0
Octacosanol	21.127	8.5	ng/ul	3377400	5	21.433	7906520	20.0
(DEL) Alkane: S...	24.521	4.2	ng/ul	1551470	6	23.910	7407020	20.0
D:C-Friedo-B':A...	28.986	20.5	ng/ul	7592760	6	23.910	7407020	20.0